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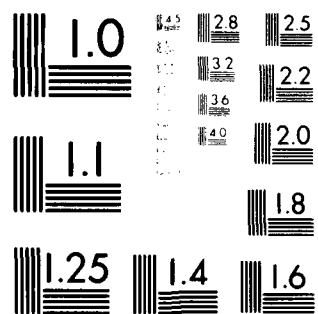
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THE ROSCOE MANUAL

Volume 17-1-High-Altitude Debris-Energy Deposition

Science Applications, Inc.
1200 Prospect Street
La Jolla, California 92038

30 June 1979

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Models of the high-altitude debris-energy partition and deposition have been revised for use in ROSCOE-IR. The principal motivation has been to provide for the increase to 23 from 11 species carried in the high-altitude grid chemistry. However, wherever feasible, corrections, improvements, and updat- ing of the models have been incorporated. Section 4 (UV Source Characteris- tics) and Section 9 (UV Deposition) of Volume 17 have been modified, and Section 7 (Partitioning of the Deposited Debris Energy and Consequent Species		

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20. ABSTRACT (Continued)

(Subroutine HPCHEM)) and Section 10 (Prompt Chemistry Associated with Group-X and Group-U Energy Deposition (Subroutine PCHEM)) of Volume 17 have been completely revised. The remaining sections in Volume 17 are unchanged.

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Conversion factors for U.S. customary
to metric (SI) units of measurement.

To Convert From	To	Multiply By
angstrom	meters (m)	1.000 000 X E -10
atmosphere (normal)	kilo pascal (kPa)	1.013 25 X E +2
bar	kilo pascal (kPa)	1.000 000 X E +2
barn	meter ² (m ²)	1.000 000 X E -28
British thermal unit (thermochemical)	joule (J)	1.054 350 X E +3
calorie (thermochemical)	joule (J)	4.184 000
cal (thermochemical)/cm ²	mega joule/m ² (MJ/m ²)	4.184 000 X E -2
curie	*giga becquerel (GBq)	3.700 000 X E +1
degree (angle)	radian (rad)	1.745 329 X E -2
degree Fahrenheit	degree kelvin (K)	$t_K = (t_F + 459.67)/1.8$
electron volt	joule (J)	1.602 19 X E -19
erg	joule (J)	1.000 000 X E -7
erg/second	watt (W)	1.000 000 X E -7
foot	meter (m)	3.048 000 X E -1
foot-pound-force	joule (J)	1.355 818
gallon (U. S. liquid)	meter ³ (m ³)	3.785 412 X E -3
inch	meter (m)	2.540 000 X E -2
jerk	joule (J)	1.000 000 X E +9
joule/kilogram (J/kg) (radiation dose absorbed)	Gray (Gy)	1.000 000
kilotons	terajoules	4.183
kip (1000 lbf)	newton (N)	4.448 222 X E +3
kip/inch ² (ksi)	kilo pascal (kPa)	6.894 757 X E +3
ktap	newton-second/m ² (N-s/m ²)	1.000 000 X E +2
micron	meter (m)	1.000 000 X E -6
mil	meter (m)	2.540 000 X E -5
mile (international)	meter (m)	1.609 344 X E +3
ounce	kilogram (kg)	2.834 952 X E -2
pound-force (lbs avoirdupois)	newton (N)	4.448 222
pound-force inch	newton-meter (N·m)	1.129 848 X E -1
pound-force/inch	newton/meter (N/m)	1.751 268 X E +2
pound-force/foot ²	kilo pascal (kPa)	4.788 026 X E -2
pound-force/inch ² (psi)	kilo pascal (kPa)	6.894 757
pound-mass (lbm avoirdupois)	kilogram (kg)	4.535 924 X E -1
pound-mass-foot ² (moment of inertia)	kilogram-meter ² (kg·m ²)	4.214 011 X E -2
pound-mass/foot ³	kilogram/meter ³ (kg/m ³)	1.601 846 X E +1
rad (radiation dose absorbed)	*Gray (Gy)	1.000 000 X E -2
roentgen	coulomb/kilogram (C/kg)	2.579 760 X E -4
shake	second (s)	1.000 000 X E -8
slug	kilogram (kg)	1.459 390 X E +1
torr (mm Hg, 0° C)	kilo pascal (kPa)	1.333 22 X E -1

*The becquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (Gy) is the SI unit of absorbed radiation.

A more complete listing of conversions may be found in "Metric Practice Guide E 380-74," American Society for Testing and Materials.

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SECTION 1

UV SOURCE CHARACTERISTICS

(Modification of Section 4 of Volume 17)

Subroutine EUXFIT did not require a change for ROSCOE-IR per se, but we have done so anyway so that the routine would conform to Sappenfield's 1975 report [Sa-75a] instead of the 1971 report [FS-71a] by Fajen and Sappenfield. The upgrading involves a modified formula as well as altered coefficients. We also correct an error near the end of the routine where the total hydro yield was used instead of that part of it left after the loss-cone and ion-leak portions had been removed.

Equation (26) in Volume 17 is still used with two exceptions:

1. For the second energy group, use $x = 1/K$ instead of $x = \ln K$.
2. For $K < 40$, the coefficients in Equation (26) for the first and third energy groups are given by a different set of values.

As implied in Volume 17, we again add the coefficients for the fifth and sixth energy groups given in Sa-75a to get the coefficients we use for the fifth energy group in the code.

SECTION 2

PARTITIONING OF THE DEPOSITED DEBRIS ENERGY
AND CONSEQUENT SPECIES (SUBROUTINE HPCHEM)

(Revision of Section 7 of Volume 17)

2-1 INTRODUCTION

The principal motivation in revising Subroutine HPCHEM for ROSCOE-IR has been to provide for the additional species carried in the high-altitude grid chemistry. The revision is extensive yet minimal. We retain the original philosophy of the model (based on a light-energy deposition) and employ a reasonable procedure to avoid malfunction when the model is applied to heavy energy-deposition cases. We do this by a modified procedure for limiting the total energy deposited so as to avoid complete burnout of diatomic molecules. We also correct a statement in Volume 17 for the maximum allowed elastic-energy deposition (HPEMAX).

Subroutine HPCHEM partitions the total energy lost in each cell by loss-cone, ion-leak, and CHEX particles undergoing inelastic and elastic collisions. The energy is partitioned into heavy-particle thermal, electron thermal, dissociation, ionization, excitation, and radiation. A model of heavy-particle prompt chemistry is also used to compute the changes in number densities of $N(^4S)$, $N(^2D)$, $N(^2P)$, N_2 , NO , NO_2 , O , $O_2(X^3\Sigma_g^-)$, $O_2(a^1\Delta_g)$, O_3 , CO , CO_2 , H , OH , HO_2 , H_2O , He , N^+ , N_2^+ , NO^+ , O^+ , O_2^+ , and electrons.

One of the simplifications made in depositing the heavy-particle energies is that the range-energy relation used in Subroutines DEPO and CHXDEP is based on the total mass density of a cell whereas in Subroutine HPCHEM only the neutral species are considered as targets. The modeling of the associated heavy-particle prompt chemistry is based on a speculative treatment [HM-72b, Section 6; HL-73b, Section 5], modified by the need to interface with the late-time grid chemistry. (The rationale for the heavy-particle prompt-chemistry modeling, to the extent it exists, will not be repeated here.) In this late-time chemistry, for atomic oxygen only $O(^1D)$ is accounted for (implicitly) as an

excited term. Thus, $O(^1S)$ is purposely excluded as a possible reaction product of the heavy-particle prompt chemistry.

In Tables 2-1 and 2-2 we summarize the reactions from inelastic (ionizing) and elastic (non-ionizing) collisions that are modeled in the prompt chemistry from heavy-particle energy deposition. The species density in the right-most columns are initial and not (more correctly) current values.

2-2 ESTABLISHMENT OF PARAMETERS

In Subroutine HPCHEM, before dealing explicitly with the partitioning of the species and energies from the inelastic and elastic collisions, we must take a number of preliminary steps and establish several parameters used in the modeling.

1. From the extended core storage for the cell of interest, obtain the total mass density $\rho(\text{g/cm}^3)$ and the number densities (cm^{-3}) of the neutral species.
2. For both the inelastic- and elastic-collision contributions, sum the specific energies deposited by the loss-cone (PEI and PEE), ion-leak (QEI and QEE), and CHEX (CEI and CEE) particles.

$$\epsilon_i(\text{erg/g}) = \text{PEI} + \text{QEI} + \text{CEI}$$

$$\epsilon_e(\text{erg/g}) = \text{PEE} + \text{QEE} + \text{CEE} \quad .$$

3. Compute the number density of nuclei in the neutral species.

$$A1 = [N(^4S)] + [N(^2D)] + [N(^2P)] + [O] + [H] + [He]$$

$$A2 = [N_2] + [NO] + [O_2(X)] + [O_2(a)] + [CO] + [OH]$$

$$A3 = [NO_2] + [O_3] + [CO_2] + [HO_2] + [H_2O]$$

$$n = \text{neutral-particle nuclei cm}^{-3}$$

$$= A1 + 2 \times A2 + 3 \times A3 \quad .$$

Table 2-1. Heavy-particle prompt-chemistry reactions from ionizing collisions.

Reaction	Branching Ratio*	Number of Ionizing Reactions, cm^{-3}
$\text{N}(^4\text{S}) \rightarrow \text{N}^+ + \text{e}$	1.0	$[\text{N}(^4\text{S})][\text{e}]/n$
$\text{N}(^2\text{D}) \rightarrow \text{N}^+ + \text{e}$	1.0	$[\text{N}(^2\text{D})][\text{e}]/n$
$\text{N}(^2\text{P}) \rightarrow \text{N}^+ + \text{e}$	1.0	$[\text{N}(^2\text{P})][\text{e}]/n$
$\text{N}_2 \rightarrow \left\{ \begin{array}{l} \text{N}_2^+ + \text{e} \\ \text{N}(^4\text{S}) + \text{N}^+ + \text{e} \end{array} \right.$	$\left. \begin{array}{l} a \\ b \end{array} \right\}$	$2[\text{N}_2][\text{e}]/n$
$\text{NO} \rightarrow \left\{ \begin{array}{l} \text{NO}^+ + \text{e} \\ \text{N}(^4\text{S}) + \text{O}^+ + \text{e} \\ \text{O}(^3\text{P}) + \text{N}^+ + \text{e} \end{array} \right.$	$\left. \begin{array}{l} a \\ b/2 \\ b/2 \end{array} \right\}$	$2[\text{NO}][\text{e}]/n$
$\text{NO}_2 \rightarrow \left\{ \begin{array}{l} \text{NO}_2^+ + \text{e} \rightarrow \text{NO} + \text{O} \\ \text{NO} + \text{O}^+ + \text{e} \\ \text{O}(^3\text{P}) + \text{NO}^+ + \text{e} \end{array} \right.$	$\left. \begin{array}{l} a \\ b/2 \\ b/2 \end{array} \right\}$	$3[\text{NO}_2][\text{e}]/n$
$\text{O} \rightarrow \text{O}^+ + \text{e}$	1.0	$[\text{O}][\text{e}]/n$
$\text{O}_2 \rightarrow \left\{ \begin{array}{l} \text{O}_2^+ + \text{e} \\ \text{O}(^3\text{P}) + \text{O}^+ + \text{e} \end{array} \right.$	$\left. \begin{array}{l} a \\ b \end{array} \right\}$	$2[\text{O}_2][\text{e}]/n$
$\text{O}_3 \rightarrow \left\{ \begin{array}{l} \text{O}_3^+ + \text{e} \rightarrow \text{O}_2 + \text{O} \\ \text{O}_2 + \text{O}^+ + \text{e} \\ \text{O}(^3\text{P}) + \text{O}_2^+ + \text{e} \end{array} \right.$	$\left. \begin{array}{l} a \\ b/2 \\ b/2 \end{array} \right\}$	$3[\text{O}_3][\text{e}]/n$

(continued)

* $a = 1/1.35$, $b = 0.35a$,

n = number density of nuclei in neutral particles.

Table 2-1 (Cont'd)

Reaction		Branching Ratio*	Number of Ionizing Reactions, cm ⁻³
CO →	$\text{CO}^+ + e \rightarrow \text{C} + \text{O}$	a	2[CO][e]/n
	$\text{O}(^3\text{P}) + \text{C}^+ + e$	b/2	
	$\text{C} + \text{O}^+ + \text{e}^{\text{C}}$	b/2	
CO ₂ →	$\text{CO}_2^+ + e \rightarrow \text{CO} + \text{O}$	a	3[CO ₂][e]/n
	$\text{O}(^3\text{P}) + \text{CO}^+ + e$	b/2	
	$\text{C} + \text{O}$		
H →	$\text{CO} + \text{O}^+ + e$	b/2	[H][e]/n
	$\text{H}^+ + e \rightarrow \text{H}$	1.0	
OH →	$\text{OH}^+ + e \rightarrow \text{O} + \text{H}$	a	2[OH][e]/n
	$\text{O}(^3\text{P}) + \text{H}^+ + e$	b/2	
	H		
HO ₂ →	$\text{H} + \text{O}^+ + e$	b/2	3[HO ₂][e]/n
	$\text{HO}_2^+ + e \rightarrow \text{OH} + \text{O}$	a	
	$\text{O}(^3\text{P}) + \text{OH}^+ + e$	b/4	
	$\text{O} + \text{H}$		
	$\text{OH} + \text{O}^+ + e$	b/4	
	$\text{H} + \text{O}_2^+ + e$	b/4	
	$\text{O}_2 + \text{H}^+ + e$	b/4	
H ₂ O →	$\text{H}_2\text{O}^+ + e \rightarrow \text{OH} + \text{H}$	a	3[H ₂ O][e]/n
	$\text{H} + \text{OH}^+ + e$	b/2	
	$\text{O} + \text{H}$		
	$\text{OH} + \text{H}^+ + e$	b/2	
	H		
He →	$\text{He}^+ + e \rightarrow \text{He}$	1.0	[He][e]/n

Table 2-2. Heavy-particle prompt-chemistry reactions from non-ionizing collisions.

Reaction		Branching Ratio*	Number of Fast Cascade Particles,* cm ⁻³
$N \equiv \left\{ \begin{array}{l} N(^4S) \\ + N(^2D) \\ + N(^2P) \end{array} \right\}$	<u>Slow</u>	<u>Fast</u>	
	\rightarrow	$\left\{ \begin{array}{ll} N(^4S) & 4/20 \\ N(^2D) & 10/20 \\ N(^2P) & 6/20 \end{array} \right\}$	$[N]n_c/n$
$N_2 \rightarrow$	$N(^4S) +$	$\left\{ \begin{array}{ll} N(^4S) & 4/20 \\ N(^2D) & 10/20 \\ N(^2P) & 6/20 \end{array} \right\}$	$2[N_2]n_c/n$
	$\left\{ \begin{array}{l} N(^4S) + \\ O(^3P) + \end{array} \right\}$	$\left\{ \begin{array}{ll} O(^3P) & c/2 \\ O(^1D) & d/2 \\ N(^4S) & (4/20)/2 \\ N(^2D) & (10/20)/2 \\ N(^2P) & (6/20)/2 \end{array} \right\}$	$2[NO]n_c/n$
$NO_2 \rightarrow$	$\left\{ \begin{array}{l} NO + \\ O(^3P) + \end{array} \right\}$	$\left\{ \begin{array}{ll} O(^3P) & c/2 \\ O(^1D) & d/2 \\ NO & 1/2 \end{array} \right\}$	$3[NO_2]n_c/n$
(continued)			

*c = 9/14, d = 5/14,

n_c = number density of particles in cascade of elastic-collision energy.

Table 2-2. (Cont'd)

Reaction		Branching Ratio*		Number of Fast Cascade Particles,* cm ⁻³	
	<u>Slow</u>	<u>Fast</u>			
O	→	$\left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \end{array} \right.$	$\left\{ \begin{array}{l} c \\ d \end{array} \right.$		$[\text{O}]n_c/n$
O ₂	$\equiv \left\{ \begin{array}{l} \text{O}_2(\text{X}) \\ +\text{O}_2(\text{a}) \end{array} \right\} \rightarrow \text{O}(^3\text{P})$	$+ \left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \end{array} \right.$	$\left\{ \begin{array}{l} c \\ d \end{array} \right.$		$2[\text{O}_2]n_c/n$
O ₃	→	$\left\{ \begin{array}{l} \text{O}_2 + \text{O}(^3\text{P}) \\ \text{O}(^3\text{P}) + \text{O}_2 \end{array} \right.$	$\left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \\ \text{O}_2 \end{array} \right.$	$\left\{ \begin{array}{l} c/2 \\ d/2 \\ 1/2 \end{array} \right.$	$3[\text{O}_3]n_c/n$
CO	→	$\left\{ \begin{array}{l} \text{C} + \text{O}(^3\text{P}) \\ \text{O}(^3\text{P}) + \text{C} \end{array} \right.$	$\left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \\ \text{C} \end{array} \right.$	$\left\{ \begin{array}{l} c/2 \\ d/2 \\ 1/2 \end{array} \right.$	$2[\text{CO}]n_c/n$
CO ₂	→	$\left\{ \begin{array}{l} \text{CO} + \text{O}(^3\text{P}) \\ \text{O}(^3\text{P}) + \text{CO} \end{array} \right.$	$\left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \\ \text{CO} \end{array} \right.$	$\left\{ \begin{array}{l} c/2 \\ d/2 \\ 1/2 \end{array} \right.$	$3[\text{CO}_2]n_c/n$
H	→	H		1.0	$[\text{H}]n_c/n$
OH	→	$\left\{ \begin{array}{l} \text{H} + \text{O}(^3\text{P}) \\ \text{O}(^3\text{P}) + \text{H} \end{array} \right.$	$\left\{ \begin{array}{l} \text{O}(^3\text{P}) \\ \text{O}(^1\text{D}) \\ \text{H} \end{array} \right.$	$\left\{ \begin{array}{l} c/2 \\ d/2 \\ 1/2 \end{array} \right.$	$2[\text{OH}]n_c/n$

(continued)

Table 2-2. (Cont'd)

Reaction		Branching Ratio*	Number of Cascade Particles,* cm ⁻³
	<u>Slow</u>	<u>Fast</u>	
HO ₂	→ {	OH + {	} 3[HO ₂]n _c /n
		O(³ P) + OH	
		H + O ₂	
		O ₂ + H	
H ₂ O	→ {	OH + H	} 3[H ₂ O]n _c /n
		H + OH	
He	→	He	[He]n _c /n

4. Compute the threshold-energy parameter used in modeling the cascade of elastic energy.

$$[N] = [N(^4S)] + [N(^2D)] + [N(^2P)]$$

$$[O_2] = [O_2(X^3\Sigma_g^-)] + [O_2(a^1\Delta_g)]$$

$$E_t = \{28.44[N] + 39.04[N_2] + 26.04[NO] + 12.48[NO_2] + 23.4[O]$$

$$+ 20.48[O_2] + 4.20[O_3] + 44.44[CO] + 21.80[CO_2]$$

$$+ 22.0[H] + 17.60[OH] + 9.40[HO_2]$$

$$+ 20.48[H_2O] + 40.00[He]\}/n .$$

In this equation the coefficient of $[O]$ includes the replacement of $\epsilon_m(O)$ by $\epsilon_m(O) + \epsilon_r(O)$ in Eq. (68) of HM-72b (or Eq. (40) of HL-73b). A similar remark applies to the other atomic species. Values of the parameters used are given in Table 2-3.

5. Compute the weighted value of the energy removed per collision in the cascade of elastic energy.

$$\epsilon(eV) = \{14.22[N] + 47.96[N_2] + 29.94[NO] + 21.64[NO_2]$$

$$+ 11.70[O] + 31.64[O_2] + 23.5[O_3] + 45.62[CO]$$

$$+ 34.30[CO_2] + 11[H] + 30.20[OH] + 23.40[HO_2]$$

$$+ 30.24[H_2O] + 20[He]\}/n .$$

6. It is necessary to limit the deposited specific energies to values less than those required, according to the model, for complete ionization and (effective) dissociation of the neutral-particle densities. In establishing such a limit one needs to recognize that the model used here for partitioning the deposited debris kinetic energy is a linearized theory and hence more appropriate for a light than heavy deposition of energy. The probability for destruction of an ambient target particle is assumed to be proportional to the initial (and not a current) density of the particular target species. This probability is also weighted by the number of nuclei in the target particle. That is, the cross section for destruction is assumed to be proportional to

Table 2-3. Parameters for the idealized cascade of elastic-collision energy and ionization energy (eV).

Particle	ϵ_d	ϵ_m	ϵ_r	$\epsilon_d + \epsilon_m + \epsilon_r$	ϵ_i
N	-	2.22 ^e	12	14.22	14.53
N ₂	9.76	2.22 ^e	12	23.98	15.58
NO	6.51	1.46 ^g	7	14.97	9.27
NO ₂	3.12 (NO - O)	0.70 ^f	7	10.82	9.78
O	-	0.70 ^f	11	11.70	13.62
O ₂	5.12	0.70 ^f	10	15.82	12.06
O ₃	1.05 (O ₂ - O)	0.70 ^f	10	11.75	12.80
CO	11.11	0.70 ^f	11	22.81	14.01
CO ₂	5.45 (O - O)	0.70 ^f	11	17.15	13.77
H	-	-	11	11	13.60
OH	4.40	0.70 ^f	10	15.1	12.94
HO ₂	$\left\{ \begin{array}{l} 2.71 \text{ (HO - O)} \\ 1.99 \text{ (H - O}_2\text{)} \\ \bar{\epsilon}_d = 2.35 \end{array} \right\}$	0.35 ^h	9	11.7	11.53
H ₂ O	5.12 (H - OH)	-	10	15.12	12.62
He	-	-	10	20	24.59

^e From (10/20) 2.37 + (6/20) 3.56 = 2.22.

^f From (5/14) 1.96 = 0.70.

^g From the mean of the values for e and f.

^h From 1/2 of the value for f.

the number of atoms in the target particle. Hence, diatomic and triatomic particles are destroyed more quickly than the atomic particles. The combination of this feature and the linearized theory would allow the diatomics and triatomics to be over-burned out if the deposited energy were limited on an energetic basis alone, i.e., if one were to use the limit

$$[e] + n_c \leq N_{HP}$$

where $[e]$ is the electron density produced by the inelastic collisions, n_c is the number density of particles in the cascade of elastic energy, and N_{HP} is the number density of ambient neutral particles. With this limit the diatomics and triatomics would be over-burned out by the factors $N_{HP}/(n/2)$ and $N_{HP}/(n/3)$, respectively. We have elected to limit the energy deposition to avoid burnout of the diatomics, to prevent certain difficulties in Subroutine PCHEM which occur if the initial value of $[N_2]$ is zero. By barely preventing the burnout of diatomics, we do allow the over-burnout of triatomics, which we correct by setting the triatomic species number densities to zero. However, this error is negligible since the triatomic species number densities are very small in the altitude region in which these effects occur.

The other possible procedures include (1) using target-independent cross-sections (which seems unrealistic) or (2) avoiding linearized theory by integrating the appropriate differential equations. Since the model was already complete except for the feature of limiting the deposited energy, neither of these two possibilities was attractive.

We now summarize our procedure for limiting the energy deposition.

Define

$$N_{HP}(\text{cm}^{-3}) = A1 + A2 + A3$$

$$\epsilon_{imax} = 28.5 \epsilon_1 N_{HP} \text{ erg/g}$$

$$\epsilon_{emax} = \frac{3}{4} (E_t + \epsilon) \epsilon_1 N_{HP} \text{ erg/g}$$

where the conversion factor ϵ_1 is

$$\epsilon_1(\text{erg eV}^{-1} \text{ cm}^3 \text{ g}^{-1}) = \epsilon_0 / \rho$$

$$\epsilon_0 = 1.60 \times 10^{-12} \text{ erg/eV}.$$

The total mass density, ρ , is appropriate here because ϵ_i and ϵ_e are computed for the total mass density. The fractions of N_{HP} destroyed by inelastic and by elastic processes (on an energetic basis, alone) are, respectively,

$$g_i = \epsilon_i / \epsilon_{imax}$$

and

$$g_e = \epsilon_e / \epsilon_{emax} .$$

If

$$F \equiv N_{HP}(g_i + g_e)/(n/2) > 0.99 ,$$

one must reduce ϵ_i and ϵ_e by the factor $0.99/F$.

2-3 INELASTIC COLLISIONS

We are now ready to deal explicitly with the inelastic collisions.

1. Compute the electron density:

$$[e] = \epsilon_i / (28.5 \epsilon_1) .$$

2. Partition the charged species from inelastic collisions.

$$[N^+]_i = \{b^{-1}[N] + 2[N_2] + [NO]\} b[e]/n$$

$$[N_2^+]_i = 2[N_2] a[e]/n$$

$$[NO^+]_i = \{2[NO] + 1.5(b/a)[NO_2]\} a[e]/n$$

$$[O^+]_i = \{[NO] + [CO] + [OH] + 1.5([NO_2] + [O_3] + [CO_2]) \\ + b^{-1}[O] + 2[O_2] + 0.75[HO_2]\} b[e]/n$$

$$[O_2^+]_i = \{2[O_2] + 1.5(b/a)([O_3] + 0.5[HO_2])\} a[e]/n .$$

3. 3.1 Record the corresponding neutral-particle densities produced by dissociative ionization in inelastic collisions:

$$[N(^4S)]_{di} = \{2[N_2] + [NO]\} b[e]/n$$

$$[\text{NO}]_{\text{di}} = [\text{NO}_2] 1.5 b[e]/n$$

$$[\text{O}]_{\text{di}} = \{[\text{NO}] + [\text{CO}] + [\text{OH}] + 1.5([\text{NO}_2] + [\text{O}_3] + [\text{CO}_2]) \\ + 2[\text{O}_2] + 0.75[\text{HO}_2]\} b[e]/n$$

$$[\text{O}_2]_{\text{di}} = \{[\text{O}_3] + 0.5[\text{HO}_2]\} 1.5 b[e]/n$$

$$[\text{CO}]_{\text{di}} = [\text{CO}_2] 1.5 b[e]/n$$

$$[\text{H}]_{\text{di}} = \{[\text{OH}] + 0.75[\text{HO}_2] + 1.5[\text{H}_2\text{O}]\} b[e]/n$$

$$[\text{OH}]_{\text{di}} = \{0.5[\text{HO}_2] + [\text{H}_2\text{O}]\} 1.5 b[e]/n$$

$$[\text{C}]_{\text{di}} = [\text{CO}] b[e]/n$$

- 3.2 Prescribe prompt recombination for those ions not carried in the late-time grid chemistry, as shown in Table 2-4.
- 3.3 Record the neutral-particle densities corresponding to these recombinations.

$$[\text{NO}]_{\text{r}} = [\text{NO}_2] 3a[e]/n$$

$$[\text{O}]_{\text{r}} = \{3([\text{NO}_2] + [\text{O}_3] + (1+b/4a)[\text{HO}_2] + (b/2a)[\text{H}_2\text{O}] \\ + (1+b/2a)[\text{CO}_2]) + 2([\text{OH}] + [\text{CO}])\} a[e]/n$$

$$[\text{O}_2]_{\text{r}} = [\text{O}_3] 3a[e]/n$$

$$[\text{CO}]_{\text{r}} = [\text{CO}_2] 3a[e]/n$$

$$[\text{H}]_{\text{r}} = \{(2+b/a)[\text{OH}] + a^{-1}(1.5 b[\text{HO}_2] + [\text{H}]) \\ + 3(1+b/a)[\text{H}_2\text{O}]\} a[e]/n$$

$$[\text{OH}]_{\text{r}} = \{[\text{HO}_2] + [\text{H}_2\text{O}]\} 3a[e]/n$$

Table 2-4. Prescribed prompt recombination of (minor) charged species not carried in late-time grid chemistry.

Reaction	Branching Ratio*	Number of Reactions cm^{-3}
$\text{NO}_2^+ + e \rightarrow \text{NO} + \text{O}$	a	$3[\text{NO}_2] [e]/n$
$\text{O}_3^+ + e \rightarrow \text{O}_2 + \text{O}$	a	$3[\text{O}_3] [e]/n$
$\text{OH}^+ + e \rightarrow \text{O} + \text{H}$	a	$2[\text{OH}] [e]/n$
	b/4	$3[\text{HO}_2] [e]/n$
	b/2	$3[\text{H}_2\text{O}] [e]/n$
$\text{H}^+ + e \rightarrow \text{H}$	b/2	$2[\text{OH}] [e]/n$
	b/4	$3[\text{HO}_2] [e]/n$
	b/2	$3[\text{H}_2\text{O}] [e]/n$
	1.0	$[\text{H}] [e]/n$
$\text{HO}_2^+ + e \rightarrow \text{OH} + \text{O}$	a	$3[\text{HO}_2] [e]/n$
$\text{H}_2\text{O}^+ + e \rightarrow \text{OH} + \text{H}$	a	$3[\text{H}_2\text{O}] [e]/n$
$\text{CO}_2^+ + e \rightarrow \text{CO} + \text{O}$	a	$3[\text{CO}_2] [e]/n$
$\text{CO}^+ + e \rightarrow \text{C} + \text{O}$	b/2	$3[\text{CO}_2] [e]/n$
	a	$2[\text{CO}] [e]/n$
$\text{C}^+ + e \rightarrow \text{C}$	b/2	$2[\text{CO}] [e]/n$
$\text{He}^+ + e \rightarrow \text{He}$	1.0	$[\text{He}] [e]/n$

* $a = 1/1.35$, $b = 0.35a$.

$$[\text{He}]_r = [\text{He}] [e]/n$$

$$[\text{C}]_r = \{(2+b/a)[\text{CO}] + (3b/2a)[\text{CO}_2]\} a[e]/n .$$

- 3.4 Record the decrease in electron density corresponding to these prescribed recombinations.

$$[e]_r = -\{3([\text{NO}_2] + [\text{O}_3] + (1+b/2a)([\text{HO}_2] + [\text{CO}_2]) \\ + (1+b/a)[\text{H}_2\text{O}]) + (2+b/a)([\text{OH}] + [\text{CO}]) \\ + a^{-1}([\text{H}] + [\text{He}]))\} a[e]/n .$$

- 3.5 Record the densities of the molecular ions in Table 2-4.

$$[\text{NO}_2^+]_r = [\text{NO}_2] 3a[e]/n$$

$$[\text{O}_3^+]_r = [\text{O}_3] 3a[e]/n$$

$$[\text{OH}^+]_r = \{2[\text{OH}] + (3b/2a)(0.5[\text{HO}_2] + [\text{H}_2\text{O}])\} a[e]/n$$

$$[\text{HO}_2^+]_r = [\text{HO}_2] 3a[e]/n$$

$$[\text{H}_2\text{O}^+]_r = [\text{H}_2\text{O}] 3a[e]/n$$

$$[\text{CO}_2^+]_r = [\text{CO}_2] 3a[e]/n$$

$$[\text{CO}^+]_r = \{2[\text{CO}] + (3b/2a)[\text{CO}]\} a[e]/n .$$

- 3.6 Compute and collate the changes in neutral species densities for inelastic collisions.

$$\delta[\text{N}(^4\text{S})]_i = -[\text{N}(^4\text{S})] \frac{[e]}{n} + [\text{N}(^4\text{S})]_{di}$$

$$\delta[\text{N}(^2\text{D})]_i = -[\text{N}(^2\text{D})] \frac{[e]}{n}$$

$$\delta[\text{N}(^2\text{P})]_i = -[\text{N}(^2\text{P})] \frac{[e]}{n}$$

$$\delta[\text{N}_2]_i = -2[\text{N}_2] \frac{[e]}{n}$$

$$\delta[\text{NO}]_i = -2[\text{NO}] \frac{[e]}{n} + [\text{NO}]_{di} + [\text{NO}]_r$$

$$\delta[\text{NO}_2]_i = -3[\text{NO}_2] \frac{[e]}{n}$$

$$\delta[\text{O}]_i = -[\text{O}] \frac{[e]}{n} + [\text{O}]_{di} + [\text{O}]_r$$

$$\delta[\text{O}_2]_i = -2[\text{O}_2] \frac{[e]}{n} + [\text{O}_2]_{di} + [\text{O}_2]_r$$

$$\delta[\text{O}_3]_i = -3[\text{O}_3] \frac{[e]}{n}$$

$$\delta[\text{CO}]_i = -2[\text{CO}] \frac{[e]}{n} + [\text{CO}]_{di} + [\text{CO}]_r$$

$$\delta[\text{CO}_2]_i = -3[\text{CO}_2] \frac{[e]}{n}$$

$$\delta[\text{H}]_i = -[\text{H}] \frac{[e]}{n} + [\text{H}]_{di} + [\text{H}]_r$$

$$\delta[\text{OH}]_i = -2[\text{OH}] \frac{[e]}{n} + [\text{OH}]_{di} + [\text{OH}]_r$$

$$\delta[\text{HO}_2]_i = -3[\text{HO}_2] \frac{[e]}{n}$$

$$\delta[\text{H}_2\text{O}]_i = -3[\text{H}_2\text{O}] \frac{[e]}{n}$$

$$\delta[\text{He}]_i = 0.0$$

$$\delta[\text{C}]_i = [\text{C}]_{di} + [\text{C}]_r .$$

3.7 The changes in charged species, so far, are:

$$\delta[\text{N}^+] = [\text{N}^+]_i$$

$$\delta[\text{N}_2^+] = [\text{N}_2^+]_i$$

$$\delta[\text{NO}^+] = [\text{NO}^+]_i$$

$$\delta[O^+] = [O^+]_i$$

$$\delta[O_2^+] = [O_2^+]_i$$

$$\delta[e] = [e] + [e]_r$$

- 3.8 Compute the sums of changes in densities of nitrogen, oxygen, carbon, and hydrogen nuclei and of charged species as measures of conservation errors.

$$\begin{aligned}\Sigma \delta N_i &= \delta[N(^4S)]_i + \delta[N(^2D)]_i + \delta[N(^2P)]_i \\ &+ \delta[NO]_i + \delta[NO_2]_i + \delta[N^+]_i + \delta[NO^+]_i \\ &+ 2\{\delta[N_2]_i + \delta[N_2^+]_i\}\end{aligned}$$

$$\begin{aligned}\Sigma \delta O_i &= \delta[NO]_i + \delta[O]_i + \delta[CO]_i + \delta[OH]_i + \delta[H_2O]_i \\ &+ \delta[NO^+]_i + [O^+]_i \\ &+ 2\{\delta[NO_2]_i + \delta[O_2]_i + \delta[CO_2]_i + \delta[HO_2]_i \\ &+ \delta[O_2^+]_i\} + 3\delta[O_3]_i\end{aligned}$$

$$\Sigma \delta C_i = \delta[CO]_i + \delta[CO_2]_i + \delta[C]_i$$

$$\Sigma \delta H_i = \delta[H]_i + \delta[OH]_i + \delta[HO_2]_i + 2\delta[H_2O]_i$$

$$\begin{aligned}\Sigma \delta [Q^+ - Q^-] &= \delta[N^+] + \delta[N_2^+] + \delta[NO^+] + \delta[O^+] \\ &+ \delta[O_2^+] - \delta[e]\end{aligned}$$

4. Partition the energy from inelastic collisions into four modes and the fraction of energy in each mode.

Electron Thermal Energy:

$$E(\text{eV/cm}^3) = 1.5\{[e] + [e]_r\}$$

$$f'_{KE} = \epsilon_1 E / \epsilon_i$$

Dissociation Energy:

$$D_i(\text{eV/cm}^3) = \{9.76[\text{N}_2] + 6.51[\text{NO}] + 5.12[\text{O}_2] \\ + 11.11[\text{CO}] + 4.40[\text{OH}] + 1.5 \times (3.12[\text{NO}_2] \\ + 1.05[\text{O}_3] + 5.45[\text{CO}_2] + 2.35[\text{HO}_2] \\ + 5.12[\text{H}_2\text{O}])\} 2b[e]/n$$

$$f'_D = \epsilon_1 D_i / \epsilon_i$$

Ionization Energy:

For those ions that are not carried in the late-time grid chemistry and therefore undergo prescribed, prompt recombination, the effective 'ionization energy' corresponding to the molecular ions is the dissociation energy of the neutral particle; for the atomic ions it is zero. These facts are reflected in the coefficients of the following expression.

$$I(\text{eV/cm}^3) = 14.53[\text{N}^+]_i + 15.58[\text{N}_2^+]_i + 9.27[\text{NO}^+]_i \\ + 13.62[\text{O}^+]_i + 12.06[\text{O}_2^+]_i + 3.12[\text{NO}_2^+]_r \\ + 1.05[\text{O}_3^+]_r + 1.11[\text{CO}^+]_r + 5.45[\text{CO}_2^+]_r \\ + 4.40[\text{OH}^+]_r + 2.71[\text{HO}_2^+]_r + 5.12[\text{H}_2\text{O}^+]_r$$

$$f_I = \epsilon_1 I / \epsilon_i$$

$$I_1(\text{erg/g}) = \epsilon_1 I$$

Radiation Energy:

$$f'_R = 1 - (f'_{KE} + f'_D + f_I)$$

$$R_i(\text{eV/cm}^3) = f'_R \epsilon_i / \epsilon_1$$

2-4

ELASTIC COLLISIONS

We now deal explicitly with the elastic collisions:

1. Compute the total number density of particles from the cascade of elastic energy:

$$n_c(\text{cm}^{-3}) = \frac{\epsilon_e}{\epsilon_1 \frac{3}{4}(E_t + \epsilon)}$$

$$= \frac{4f_{KE}\epsilon_e}{\epsilon_1(3E_t - \epsilon)}$$

where

$$f_{KE} = \frac{E_t - \epsilon/3}{E_t + \epsilon}.$$

2. Partition the neutral species from elastic collisions.
 - 2.1 The fast-particle densities from the elastic-energy cascade are:

$$[N]_{f1} = [N]n_c/n$$

$$[N]_{f2} = \{2[N_2] + [NO]\} n_c/n$$

$$[N]_f = [N]_{f1} + [N]_{f2}$$

$$[NO]_f = [NO_2] 1.5n_c/n$$

$$[O]_{f1} = [O] n_c/n$$

$$[O]_{f2} = \{[NO] + 2[O_2] + [CO] + [OH]\} n_c/n$$

$$[O]_{f3} = \{[NO_2] + [O_3] + [CO_2] + 0.5[HO_2]\} 1.5 n_c/n$$

$$[O]_f = [O]_{f1} + [O]_{f2} + [O]_{f3}$$

$$[O_2]_f = \{[O_3] + 0.5[HO_2]\} 1.5 n_c/n$$

$$[CO]_f = [CO_2] 1.5 n_c/n$$

$$[H]_f = \{[H] + [OH] + 0.75[HO_2] + 1.5[H_2O]\} n_c/n$$

$$[OH]_f = \{0.5[HO_2] + [H_2O]\} 1.5 n_c/n$$

$$[He]_f = [He] n_c/n$$

$$[C]_f = [CO] n_c/n .$$

2.2 The slow-particle densities from the elastic-energy cascade are:

$$[N]_s = [N]_{f2}$$

$$[NO]_s = [NO]_f$$

$$[O]_s = [O]_{f2} + [O]_{f3}$$

$$[O_2]_s = \{[O_3] + 0.5[HO_2]\} 1.5 n_c/n$$

$$[CO]_s = [CO_2] 1.5 n_c/n$$

$$[H]_s = \{[OH] + 0.75[HO_2] + 1.5[H_2O]\} n_c/n$$

$$[OH]_s = \{0.5[HO_2] + [H_2O]\} 1.5 n_c/n$$

$$[C]_s = [CO] n_c/n .$$

2.3 Compute and collate the changes in species densities for elastic collisions.

$$\delta[N(^4S)]_e = -[N(^4S)] \frac{n_c}{n} + \frac{4}{20}[N]_f + [N]_s$$

$$\delta[N(^2D)]_e = -[N(^2D)] \frac{n_c}{n} + \frac{10}{20} [N]_f$$

$$\delta[N(^2P)]_e = -[N(^2P)] \frac{n_c}{n} + \frac{6}{20} [N]_f$$

$$\delta[N_2]_e = -2[N_2] \frac{n_c}{n}$$

$$\delta[\text{NO}]_e = -2[\text{NO}] \frac{n_c}{n} + [\text{NO}]_f + [\text{NO}]_s$$

$$\delta[\text{NO}_2]_e = -3[\text{NO}_2] \frac{n_c}{n}$$

$$\delta[\text{O}]_e = -[\text{O}] \frac{n_c}{n} + [\text{O}]_f + [\text{O}]_s$$

$$\delta[\text{O}_2]_e = -2[\text{O}_2] \frac{n_c}{n} + [\text{O}_2]_f + [\text{O}_2]_s$$

$$\delta[\text{O}_3]_e = -3[\text{O}_3] \frac{n_c}{n}$$

$$\delta[\text{CO}]_e = -2[\text{CO}] \frac{n_c}{n} + [\text{CO}]_f + [\text{CO}]_s$$

$$\delta[\text{CO}_2]_e = -3[\text{CO}_2] \frac{n_c}{n}$$

$$\delta[\text{H}]_e = -[\text{H}] \frac{n_c}{n} + [\text{H}]_f + [\text{H}]_s$$

$$\delta[\text{OH}]_e = -2[\text{OH}] \frac{n_c}{n} + [\text{OH}]_f + [\text{OH}]_s$$

$$\delta[\text{HO}_2]_e = -3[\text{HO}_2] \frac{n_c}{n}$$

$$\delta[\text{H}_2\text{O}]_e = -3[\text{H}_2\text{O}] \frac{n_c}{n}$$

$$\delta[\text{He}]_e = -[\text{He}] \frac{n_c}{n} + [\text{He}]_f$$

$$\delta[\text{C}]_e = [\text{C}]_f + [\text{C}]_s$$

2.4 Compute the sums of changes in densities of nitrogen, oxygen, carbon, and hydrogen nuclei as measures of conservation errors.

$$\begin{aligned} \Sigma \delta N_e &= \delta[\text{N}(^4\text{S})]_e + \delta[\text{N}(^2\text{D})]_e + \delta[\text{N}(^2\text{P})]_e \\ &+ [\text{NO}]_e + \delta[\text{NO}_2]_e + 2\delta[\text{N}_2]_e \end{aligned}$$

$$\begin{aligned}
\Sigma \delta O_e &= \delta[NO]_e + \delta[O]_e + \delta[CO]_e + \delta[OH]_e \\
&+ \delta[H_2O]_e + 3\delta[O_3]_e \\
&+ 2\{\delta[NO_2]_e + \delta[O_2]_e + \delta[CO_2]_e + \delta[HO_2]_e\} \\
\Sigma \delta C_e &= \delta[CO]_e + \delta[CO_2]_e + \delta[C]_e \\
\Sigma \delta H_e &= \delta[H]_e + \delta[OH]_e + \delta[HO_2]_e + 2\delta[H_2O]_e .
\end{aligned}$$

3. Partition among allowed states the (total) atomic-particle densities from the elastic-energy cascade.

$$[N(^4S)] = \frac{4}{20} [N]_f + [N]_s$$

$$[N(^2D)] = \frac{10}{20} [N]_f$$

$$[N(^2P)] = \frac{6}{20} [N]_f$$

$$[O(^3P)] = \frac{9}{14} [O]_f + [O]_s$$

$$[O(^1D)] = \frac{5}{14} [O]_f .$$

4. Partition the energy from elastic collisions into four modes.
Heavy-particle thermal energy:

$$K(\text{eV/cm}^3) = f_{KE} \epsilon_e / \epsilon_1$$

$$K_1(\text{erg/g}) = \epsilon_1 K$$

Dissociation energy:

$$D_e(\text{eV/cm}^3) = \{9.76[\text{N}_2] + 6.51[\text{NO}] + 5.12[\text{O}_2] \\ + 11.11[\text{CO}] + 4.40[\text{OH}] + 1.5(3.12[\text{NO}_2] \\ + 1.05[\text{O}_3] + 5.45[\text{CO}_2] + 2.35[\text{HO}_2] \\ + 5.12[\text{H}_2\text{O}])\} 2n_c/n$$

Excitation energy:

$$X_e(\text{eV/cm}^3) = (2.37 \times \frac{10}{20} + 3.56 \frac{6}{20})[\text{N}]_f \\ + 1.96 \times \frac{5}{14} [\text{O}]_f$$

$$X_{el}(\text{erg/g}) = \epsilon_1 X_e$$

Radiation energy:

$$R_e(\text{eV/cm}^3) = \{0.5(12[\text{N}] + 11[\text{O}] + 11[\text{H}] + 20[\text{He}]) \\ + 12[\text{N}_2] + 7[\text{NO}] + 10[\text{O}_2] + 11[\text{CO}] \\ + 10[\text{OH}] + 1.5(7[\text{NO}_2] + 10[\text{O}_3] + 11[\text{CO}_2] \\ + 9[\text{HO}_2] + 10[\text{H}_2\text{O}])\} 2n_c/n$$

2-5 COMBINED RESULTS FROM INELASTIC AND ELASTIC COLLISIONS

We can now combine the results from inelastic and elastic collisions.

1. Add the contributions from the inelastic and elastic collisions to obtain the total values of dissociation and radiation energies.

$$D(\text{eV/cm}^3) = D_i + D_e$$

$$D_1(\text{erg/g}) = \epsilon_1 D$$

$$R(\text{eV}/\text{cm}^3) = R_1 + R_e$$

$$R_1(\text{erg/g}) = \epsilon_1 R$$

2. Compute the total fractional partitions of energy for the six modes.

$$f_K = \epsilon_1 K / (\epsilon_i + \epsilon_e)$$

$$f_E = \epsilon_1 E / (\epsilon_i + \epsilon_e)$$

$$f_D = \epsilon_1 D / (\epsilon_i + \epsilon_e)$$

$$f_{X_e} = \epsilon_1 X_e / (\epsilon_i + \epsilon_e)$$

$$f_I = \epsilon_1 I / (\epsilon_i + \epsilon_e)$$

$$f_R = \epsilon_1 R / (\epsilon_i + \epsilon_e)$$

The fractional error in energy conservation is

$$F = f_K + f_E + f_D + f_{X_e} + f_I + f_R - 1$$

3. Compute the changes in species densities for both inelastic and elastic collisions.

$$\delta[N(^4S)] = \delta[N(^4S)]_i + \delta[N(^4S)]_e$$

$$\delta[N(^2D)] = \delta[N(^2D)]_i + \delta[N(^2D)]_e$$

$$\delta[N(^2P)] = \delta[N(^2P)]_i + \delta[N(^2P)]_e$$

$$\delta[N_2] = \delta[N_2]_i + \delta[N_2]_e$$

$$\delta[NO] = \delta[NO]_i + \delta[NO]_e$$

$$\delta[NO_2] = \delta[NO_2]_i + \delta[NO_2]_e$$

$$\delta[O] = \delta[O]_i + \delta[O]_e$$

$$\delta[O_2] = \delta[O_2]_i + \delta[O_2]_e$$

$$\delta[O_2(X)] = \delta[O_2] [O_2(X)]/[O_2]$$

$$\delta[O_2(a)] = \delta[O_2] \{1 - [O_2(X)]/[O_2]\}$$

$$\delta[O_3] = \delta[O_3]_i + \delta[O_3]_e$$

$$\delta[CO] = \delta[CO]_i + \delta[CO]_e$$

$$\delta[CO_2] = \delta[CO_2]_i + \delta[CO_2]_e$$

$$\delta[H] = \delta[H]_i + \delta[H]_e$$

$$\delta[OH] = \delta[OH]_i + \delta[OH]_e$$

$$\delta[HO_2] = \delta[HO_2]_i + \delta[HO_2]_e$$

$$\delta[H_2O] = \delta[H_2O]_i + \delta[H_2O]_e$$

$$\delta[He] = \delta[He]_i + \delta[He]_e$$

$$\delta[C] = \delta[C]_i + \delta[C]_e$$

4. Compute the sums of changes in densities of nitrogen, oxygen, carbon, and hydrogen nuclei as measures of conservation errors.

$$\Sigma \delta N = \Sigma \delta N_i + \Sigma \delta N_e$$

$$\Sigma \delta O = \Sigma \delta O_i + \Sigma \delta O_e$$

$$\Sigma \delta C = \Sigma \delta C_i + \Sigma \delta C_e$$

$$\Sigma \delta H = \Sigma \delta H_i + \Sigma \delta H_e$$

5. Compute the sum of electron thermal and $O(^1D)$ excitation energies per newly-formed electron.

$$E_{pe}(\text{eV/electron}) = \{E + 1.96(5/14)[O]\} \delta[e] .$$

6. Store changes in cell quantities in temporary scratch area (BUF2).

$$\text{BUF2}(1) = \delta[N(^4S)]$$

$$\text{BUF2}(14) = \delta[OH]$$

$$\text{BUF2}(2) = \delta[N(^2D)]$$

$$\text{BUF2}(15) = \delta[HO_2]$$

$$\text{BUF2}(3) = \delta[N(^2P)]$$

$$\text{BUF2}(16) = \delta[H_2O]$$

$$\text{BUF2}(4) = \delta[N_2]$$

$$\text{BUF2}(17) = \delta[He]$$

$$\text{BUF2}(5) = \delta[NO]$$

$$\text{BUF2}(18) = \delta[N^+]$$

$$\text{BUF2}(6) = \delta[NO_2]$$

$$\text{BUF2}(19) = \delta[N_2^+]$$

$$\text{BUF2}(7) = \delta[O]$$

$$\text{BUF2}(20) = \delta[NO^+]$$

$$\text{BUF2}(8) = \delta[O_2(X)]$$

$$\text{BUF2}(21) = \delta[O^+]$$

$$\text{BUF2}(9) = \delta[O_2(a)]$$

$$\text{BUF2}(22) = \delta[O_2^+]$$

$$\text{BUF2}(10) = \delta[O_3]$$

$$\text{BUF2}(23) = \delta[e]$$

$$\text{BUF2}(11) = \delta[CO]$$

$$\text{BUF2}(24) = E_{pe}$$

$$\text{BUF2}(12) = \delta[CO_2]$$

$$\text{BUF2}(25) = K_1 .$$

$$\text{BUF2}(13) = \delta[H]$$

SECTION 3

UV DEPOSITION

(Modification of Section 9 of Volume 17)

3-1 INTRODUCTION

The total computation of UV deposition requires six major subroutines, as noted in Section 9 of Volume 17. Here we give a very brief overview and guide to the changes in those subroutines.

The modifications to Subroutine EUXFIT have been described in Section 1. Subroutine PLINE now distinguishes between $N(^4S)$ and $N(^2D)$ in the zeroing of line integrals performed in Subroutine PINT. Subroutine PINT now distinguishes between $N(^4S)$ and $N(^2D)$ in forming the line integrals of the species densities. Subroutine BEDGE now distinguishes between $N(^4S)$ and $N(^2D)$ in determining the radius to the B-edge. Subroutine PHEAT now provides for all the additional species in ROSCOE-IR and for $N(^2D)$ as an attenuator of Group-U fluences. The extensive changes to Subroutine PCHEM are described in Section 4.

3-2 SUBROUTINE PLINE (Modification of Section 9.1.8.c of Volume 17)

A new integral (SNDINT) has been introduced to pertain to a newly-carried species, $N(^2D)$. This new integral is to be distinguished from the old integral (SNINT) which used to pertain to nitrogen atoms (N) without distinction as to the ground term, but which now pertains to $N(^4S)$.

3-3 SUBROUTINE PINT (Modification of Section 9.2 of Volume 17)

Replace the integral for SNINT by the two expressions

$$SNINT = \int_0^{SRN} [N(^4S)] dr, \text{ cm}^{-2}$$

$$SNDINT = \int_0^{SRN} [N(^2D)] dr, \text{ cm}^{-2} .$$

Over a ray segment between SR and SRN, the corresponding contributions to these two integrals are DSN4SI and DSN2DI, respectively. SPECIE(I) now denotes the concentration of N_2 , O_2 , $N(^4S)$, O, and $N(^2D)$, respectively, for $I = 1, 2, 3, 4$, and 5.

On page 89 of Volume 17, DRHOI is misspelled as DHROI.

3-4 SUBROUTINE BEDGE

3-4.1 Modification of Section 9.3.1 of Volume 17

The old line integral SNU of the density of species N has been replaced by the two line integrals SNU and SNDU for the species $N(^4S)$ and $N(^2D)$, respectively.

3-4.2 Modification of Section 9.3.2 of Volume 17

The index I in SPECIE(I) now denotes the species N_2 , O_2 , $N(^4S)$, O, and $N(^2D)$, respectively, for $I = 1, 2, 3, 4$, and 5.

3-4.3 Modification of Section 9.3.3 of Volume 17

In Figure 20 on page 94 of Volume 17, SPECIE(3) is replaced by the sum (SPECIE(3) + SPECIE(5)) in computing EVEN, RHOSUM, and XMUBAR. On page 96 there is the additional line integral,

$$SNDU = SNDINT + SPECIE(5) * DEL - DSNDI,$$

and the sum over J is extended from $J = 1, 4$ to $J = 1, 5$ in computing XMUBAR.

3-5 SUBROUTINE PHEAT (Modification of Section 9.4 of Volume 17)

The sum over J is extended from $J = 1, 4$ to $J = 1, 5$ in computing SUMIN(L), SUMOUT(L), PEFBAR(L), FLUX(L), and XMU(L). See formulas in Section 9.4.1 and in 9.4.3 of Volume 17 (pages 98, 99).

SECTION 4

PROMPT CHEMISTRY ASSOCIATED WITH GROUP-X AND GROUP-U ENERGY DEPOSITION (SUBROUTINE PCHEM)

(Revision of Section 10 of Volume 17)

4-1 INTRODUCTION

Subroutine PCHEM has been extensively revised in detail but not in overall structure in going from ROSCOE-Radar to ROSCOE-IR. New provisions in Subroutine PCHEM include:

1. The additional species for ROSCOE-IR.
2. An increase to 25 from 12 inputs from the BUF2 array, corresponding to the altered output from Subroutine HPCHEM.
3. A revised procedure for computing the ionization and species densities resulting from the Group-X energy deposition (computed in Subroutine PHEAT). Included are dissociative ionization of N_2 and O_2 , species and excited states resulting from non-ionizing collisions, and an improved treatment of CO_2 destruction with protection against abortion, when $[N_2]$ is very small. The other nine minor species are also treated.
4. A revised procedure for computing the ionization and species densities resulting from the Group-U energy deposition. The excited-state species $N(^2D)$ is now included in the line integrals (performed in Subroutine PLINE) affecting the Group-U fluences. Group-U absorption cross-sections are provided for each of the 17 following listed neutral species that were originally designated to be included in the ROSCOE-IR grid chemistry,

<u>I</u>	<u>Species</u>	<u>I</u>	<u>Species</u>	<u>I</u>	<u>Species</u>
1	N_2	7	NO	13	HO_2
2	$O_2(X)$	8	NO_2	14	H_2O
3	$N(^4S)$	9	$O_2(a)$	15	CO_2
4	O	10	O_3	16	CO
5	$N(^2D)$	11	H	17	He
6	$N(^2P)$	12	OH		

However, owing to the limited types of ions carried in the grid chemistry (N_2^+ , NO^+ , O_2^+ , N^+ , O^+), we prescribe prompt dissociative recombination for molecular ions and radiative recombination for atomic ions not carried in the grid chemistry.

5. An increase to 35 from 18 outputs in the BUF1 array.

As in ROSCOE-Radar, Subroutine PCHEM first combines (a) the changes in species densities due to debris deposition, computed in Subroutine HPCHEM, with (b) the previous species densities of a cell and then computes the ionization and species densities from the Group-X and Group-U energy depositions.

Subroutine PCHEM still contains numerous compromises and adjustments made necessary by using energy deposition models that are (a) instantaneous and (b) mismatched with the late-time chemistry modules, although numerous improvements have been made.

4-2 DETERMINATION OF INITIAL SPECIES FOR COMPUTING THE PROMPT CHEMISTRY ASSOCIATED WITH GROUP-X AND GROUP-U ENERGY DEPOSITIONS

Before computing the prompt chemistry associated with the energy depositions of Groups X and U, we must combine the changes in species densities due to debris deposition with the previous species densities.

The changes in the species densities and electronic thermal and excitation energy are stored in the BUF2 array by Subroutine HPCHEM. The number of these variables, defined in Table 4-1, has increased to 25 for ROSCOE-IR from 12 for ROSCOE-Radar. These quantities are appropriately combined with those from the BUF array to get the starting conditions for the Group-X and Group-U energy depositions. We check charge balance (by taking the difference between positive ions and electrons) after combining the HPCHEM-computed changes in species densities with the previous densities of the cells.

Table 4-1. Inputs to subroutine PCHEM from BUF2 array for those cell quantities updated by Subroutine HPCHEM as a result of debris deposition.

I	BUF2(I)
1	Change in $[N(^4S)]$, cm^{-3}
2	Change in $[N(^2D)]$, cm^{-3}
3	Change in $[N(^2P)]$, cm^{-3}
4	Change in $[N_2]$, cm^{-3}
5	Change in $[NO]$, cm^{-3}
6	Change in $[NO_2]$, cm^{-3}
7	Change in $[O]$, cm^{-3}
8	Change in $[O_2(X)]$, cm^{-3}
9	Change in $[O_2(a)]$, cm^{-3}
10	Change in $[O_3]$, cm^{-3}
11	Change in $[CO]$, cm^{-3}
12	Change in $[CO_2]$, cm^{-3}
13	Change in $[H]$, cm^{-3}
14	Change in $[OH]$, cm^{-3}
15	Change in $[HO_2]$, cm^{-3}
16	Change in $[H_2O]$, cm^{-3}
17	Change in $[He]$, cm^{-3}
18	Change in $[N^+]$, cm^{-3}
19	Change in $[N_2^+]$, cm^{-3}
20	Change in $[NO^+]$, cm^{-3}
21	Change in $[O^+]$, cm^{-3}
22	Change in $[O_2^+]$, cm^{-3}
23	Change in $[e]$, cm^{-3}
24	Change in electron thermal energy and $O(^1D)$ excitation energy per newly-formed electron, eV/electron
25	Change in heavy-particle thermal energy, erg/g

4-3 IONIZATION AND SPECIES DENSITIES FROM GROUP-X DEPOSITION

4-3.1 Introduction

The computation of the species densities from Group-X deposition was described in Volume 17 as being done very simply. The current computation is quite complex, resulting partly from treating additional species required for IR and partly from attempting to make the computation more realistic for both radar and IR purposes.

To facilitate relating this text to the coding, we describe the major steps in performing the overall calculation. Some steps are simple enough that no further explanation is required. In other cases the steps are more subtle and deserve explanatory information. Sometimes we will provide such information as we proceed; at other times we will refer to Appendix A for more extensive background information.

4-3.2 The Major Steps

1. Sum the N, O, C, and H nuclei densities for later use in mass-conservation checks.
2. Preset certain variables pertaining to Group-U deposition. (While this step has nothing to do with Group-X deposition per se, it provides for the possibility that a Case-2 cell follows either a Case-1 or a Case-3 cell. For a Case-2 cell, no computation is made of species resulting from Group-X deposition.)
3. 3.1 Use the specific energy absorbed from Group-X deposition (DAIXX(erg/g)) computed in Subroutine PHEAT and the mass density (RHO(g/cm³)) to get the corresponding energy density (DELEX(eV/cm³)).

$$\text{DELEX} = \text{DAIXX} \times \text{RHO} / (1.6 \times 10^{-12}) \quad (1)$$

- 3.2 Determine the fraction (FNEUT) of the absorbed energy to be assigned to deposition in the neutral-particle gas. (Here we consider only the species N, N₂, NO, O, O₂, N⁺, N₂⁺, NO⁺, O⁺, and O₂⁺.) The prescription we adopted to compute FNEUT is described in Section A-2.2.2, where FNEUT is denoted by f_n. One evaluates Equation (A15) with use of Equations (A16) and (A17) and the parameters in Table A-4.

4. 4.1 Replace the value used in Volume 17 for the energy per ion pair, 35 eV per ion pair, by a computed value (EIP) that depends on the mix of selected neutral particles ($s = N, N_2, NO, O, \text{ and } O_2$), as described in Section A-2.2.4. Use Equation (A18),

$$EIP \equiv E_{ip} = \sum_s f_s E_{ip}(s), \quad (2)$$

where the fractions f_s characterize the mix for the particles,

$$f_s = [s] / \sum_s [s]. \quad (3)$$

The parameters $E_{ip}(s)$ are given in Table A-4.

- 4.2 Compute the ion-pair density:

$$AIPX(ip/cm^3) \equiv IP = DELEX \times FNEUT/EIP. \quad (4)$$

5. 5.1 Divide all the neutral species carried in the HAG into three groups. The species in the first group are chosen because they are the principal neutral species and because we have an improved technique for computing the energy deposition. The third group is designated to facilitate a special treatment for CO_2 . Group 2 contains the remaining minor neutral species. The groups are:

Group 1: N, N_2, O, O_2

Group 2: $NO, NO_2, O_3, CO, H, OH, HO_2, H_2O, He$

Group 3: CO_2

Sum the densities $[J_k]$ in each of the three groups and also sum the group-sums:

$$SUMGP_k = \sum_{J_k} [J_k] \quad k = 1, 2, 3 \quad (5a)$$

$$SMNEUT = \sum_{k=1}^3 SUMGP_k. \quad (5b)$$

- 5.2 Set the maximum allowed ion-pair density in the neutral-particle gas, AIPXMX, by considering only the Group-1 particles. For the current model, and for considerations of late-time species, we need to set the number of J_1 -particle destructions (by collisional ionization, and for molecules, also dissociative ionization, collisional dissociation, and collisional excitation) per ion pair in a

J_1 -particle gas as $D_{ip}(J_1)$ ($J_1 = N, N_2, O, O_2$). To set these quantities we need to introduce the branching ratios (R_{N+} and R_{O+} , as in Section A-2.1) for dissociative ionization of N_2 and O_2 by electron impact and the ratios ($F_d(N_2)$ and $F_d(O_2)$, as in Section A-2.3) of collisional dissociation to collisional ionization. The quantities $D_{ip}(J_1)$, used in estimating AIPXMX, can be set as

$$D_{ip}(N) = 1 \quad D_{ip}(N_2) = 1 + (1-R_{N+})F_d(N_2) \quad (6a,b)$$

$$D_{ip}(O) = 1 \quad D_{ip}(O_2) = 1 + (1-R_{O+})F_d(O_2). \quad (6c,d)$$

Finally, we compute AIPXMX from the expression

$$AIPXMX = 0.9 \sum_{J_1} \frac{[J_1]_o}{D_{ip}(J_1)} \frac{[J_1]_o}{SUMGP_1}, \quad (7)$$

where 0.9 is an ad hoc safety factor and $J_1 = N, N_2, O, \text{ and } O_2$.

- 5.3 Initially distribute the Group-X ion-pair density among the three groups in proportion to the densities $SUMGP_k$,

$$AIPX_k = \frac{AIPX \times SUMGP_k}{\sum_k SUMGP_k}. \quad (8)$$

For Group-1 and -3 particles we will later redistribute the ion-pair density $AIPX_1 + AIPX_2$. For Group-2 particles, we simply proceed as in Volume 17 by distributing the ion-pair density $AIPX_2$ according to the relative abundance of each of the Group-2 particles.

6. Determine the altered species densities from Group-X deposition in the Group-2 particles according to the prompt-chemistry reactions assumed in Table 4-2, where $[e]_2 \equiv AIPX_2$ and $n_2 \equiv SUMGP_2$. Note that collisional ionization and dissociative ionization of the Group-2 (and Group-3) particles lead to many ions not carried in the HAG chemistry. To obviate this difficulty we prescribe immediate dissociative recombination for such molecular ions and radiative recombination for such atomic ions.

Table 4-2. Prompt-chemistry reactions assumed during x-ray deposition for Group-2 (minor species) particles.

Reaction		Branching Ratio*	Number of Ionizing Reactions,* cm ⁻³
NO	$\text{NO}^+ + e$	a	$[\text{NO}][e]_2/n_2$
	$\text{N}(^4\text{S}) + \text{O}^+ + e$	b/2	
	$\text{O} + \text{N}^+ + e$	b/2	
	$\text{N}(^4\text{S}) + \text{O}$	c	
NO_2	$\text{NO}_2^+ + e \rightarrow \text{NO} + \text{O}$	a	$[\text{NO}_2][e]_2/n_2$
	$\text{NO} + \text{O}^+ + e$	b/2	
	$\text{O} + \text{NO}^+ + e$	b/2	
	$\text{NO} + \text{O}$	c	
O_3	$\text{O}_3^+ + e \rightarrow \text{O}_2 + \text{O}$	a	$[\text{O}_3][e]_2/n_2$
	$\text{O}_2 + \text{O}^+ + e$	b/2	
	$\text{O} + \text{O}_2^+ + e$	b/2	
	$\text{O}_2 + \text{O}$	c	
CO	$\text{CO}^+ + e \rightarrow \text{C} + \text{O}$	a	$[\text{CO}][e]_2/n_2$
	$\text{O} + \underbrace{\text{C}^+ + e}_{\text{C}}$	b/2	
	$\text{C} + \text{O}^+ + e$	b/2	
	$\text{C} + \text{O}$	c	

(continued)

* a = 0.75, b = 0.25, c = 0.8,

$[e]_2$ = x-ray deposition ion-pair density assigned to Group 2,

n_2 = density of group-2 particles.

Table 4-2. (Cont'd)

		Reaction	Branching Ratio	Number of Ionizing Reactions, cm ⁻³
H	→	H ⁺ + e → H	1.0	[H][e] ₂ /n ₂
OH	→	OH ⁺ + e → O + H	a	{ [OH][e] ₂ /n ₂
		O + $\underbrace{\text{H}^+ + e}_{\text{H}}$	b/2	
		H + O ⁺ + e	b/2	
		O + H	c	
HO ₂	→	HO ₂ ⁺ + e → OH + O	a	{ [H ₂ O][e] ₂ /n ₂
		O + $\underbrace{\text{OH}^+ + e}_{\text{O+H}}$	b/4	
		OH + O ⁺ + e	b/4	
		H + O ₂ ⁺ + e	b/4	
		O ₂ + $\underbrace{\text{H}^+ + e}_{\text{H}}$	b/4	
		OH + O	c/2	
		H + O ₂	c/2	
H ₂ O	→	H ₂ O ⁺ + e → OH + H	a	{ [H ₂ O][e] ₂ /n ₂
		H + $\underbrace{\text{OH}^+ + e}_{\text{O+H}}$	b/2	
		OH + $\underbrace{\text{H}^+ + e}_{\text{H}}$	b/2	
		OH + H	c	
He	→	He ⁺ + e → He	1.0	[He][e] ₂ /n ₂

The value for the dissociative ionization branching ratio (b) is a nominal, mean value suggested by averaging $R_N^+ = 0.192$ and $R_O^+ = 0.302$. The collisional ionization branching ratio (a) is just 1-b. The collisional dissociation branching ratio (c) is suggested by averaging $[(1-R_N^+)F_d(N_2) = 1.00]$ and $[(1-R_O^+)F_d(O_2) = 0.614]$.

Before writing the changes in Group-2 particle densities we introduce several new constants:

$$F_1 = a + 0.5b \quad (9a)$$

$$F_2 = AIPX_2/SUMGP_2 \equiv [e]_2/n_2 \quad (9b)$$

$$F_3 = 1 + c \quad (9c)$$

$$F_4 = F_1 + c \quad (9d)$$

$$F_{23} = F_2 F_3 \quad (9e)$$

$$\delta_2[N(^4S)] = F_2(0.5b + c)[NO]_o \quad (10a)$$

$$\delta_2[NO] = F_2\{F_4[NO_2]_o - F_3[NO]_o\} \quad (10b)$$

$$\delta_2[NO_2] = -F_{23}[NO_2]_o \quad (10c)$$

$$\begin{aligned} \delta_2[O] = F_2\{F_4([NO_2]_o + [O_3]_o + [CO]_o + [OH]_o \\ + (F_1 + 0.5c)[HO_2]_o \\ + (0.5b + c)[NO]_o + 0.5b[H_2O]_o\} \end{aligned} \quad (10d)$$

$$\delta_2[O_2] = F_2\{F_4[O_3]_o + (0.25b + 0.5c)[HO_2]_o\} \quad (10e)$$

$$\delta_2[O_3] = -F_{23}[O_3]_o \quad (10f)$$

$$\delta_2[CO] = -F_{23}[CO]_o \quad (10g)$$

$$\begin{aligned} \delta_2[H] = F_2\{F_3[OH]_o + (0.75b + 0.5c)[HO_2]_o \\ + (a + 1.5b + c)[H_2O]_o\} \end{aligned} \quad (10h)$$

$$\delta_2[\text{OH}] = F_2\{F_4[\text{H}_2\text{O}]_0 - F_3[\text{OH}]_0 + (a + 0.25b + 0.5c)[\text{HO}_2]_0\} \quad (10i)$$

$$\delta_2[\text{HO}_2] = -F_{23}[\text{HO}_2]_0 \quad (10j)$$

$$\delta_2[\text{H}_2\text{O}] = -F_{23}[\text{H}_2\text{O}]_0 \quad (10k)$$

$$\delta_2[\text{He}] = 0 \quad (10l)$$

$$\delta_2[\text{N}^+] = F_2 \ 0.5b[\text{NO}]_0 \quad (10m)$$

$$\delta_2[\text{NO}^+] = F_2\{a[\text{NO}]_0 + 0.5b[\text{NO}_2]_0\} \quad (10n)$$

$$\delta_2[\text{O}^+] = F_2 \ 0.5b\{[\text{NO}]_0 + [\text{NO}_2]_0 + [\text{O}_3]_0 + [\text{CO}]_0 + [\text{OH}]_0 + 0.5[\text{HO}_2]_0\} \quad (10o)$$

$$\delta_2[\text{O}_2^+] = F_2 \ 0.5b\{[\text{O}_3]_0 + 0.5[\text{HO}_2]_0\} \quad (10p)$$

$$\delta_2[e] = F_2\{[\text{NO}]_0 + b([\text{NO}_2]_0 + [\text{O}_3]_0 + 0.5([\text{CO}]_0 + [\text{OH}]_0 + [\text{HO}_2]_0))\} \quad (10q)$$

$$\delta_2[\text{C}] = F_{23}[\text{CO}]_0 \quad (10r)$$

One can show analytically that the N, O, C, and H nuclei are conserved for the Group-2 reactions.

7. Treat the Group-1 and Group-3 particles by a procedure in which some of the steps are interleaved.

- 7.1 Perform the first nine of fifteen steps in treating the Group-1 particles. The background information for treating the Group-1 particles is given in Appendix A. The information in Table 4-3 will be useful in considering the first seven steps for the Group-1 particles.

Table 4-3. Ion-production reactions for Group-1 particles (N_2 , O_2 , N , O) during x-ray deposition.

Reaction		Branching Ratio	Number of Reactions* cm^{-3}
$N_2 \rightarrow$	$N_2^+ + e$	$1 - R_{N^+}$	$(S^+; e, N_2)_{ip} \text{ IP}$
	$N + N^+ + e$	R_{N^+}	
$O^+ \rightarrow$	$O_2^+ + e$	$1 - R_{O^+}$	$(S^+; e, O_2)_{ip} \text{ IP}$
	$O + O^+ + e$	R_{O^+}	
$N \rightarrow$	$N^+ + e$	1.0	$(S^+; N)_{ip} \text{ IP}$
$O \rightarrow$	$O^+ + e$	1.0	$(S^+; O)_{ip} \text{ IP}$

*The molecular reactions include the modeling of just the electron slowing-down collisions. The atomic reactions include the modeling of both the photoabsorption event and the electron slowing-down collisions. This table does not include the small number of additional N^+ and O^+ ions, included in the model, which result from the photoabsorption events in N_2 and O_2 .

Group-1 Step 1. Determine the fractional mix of the Group-1 species.

$$f_i = [i] / \sum_i [i] \quad (11)$$

$$i = N, N_2, O, O_2 .$$

Group-1 Step 2. Determine the number of ions from species i , $(S^+;i)$, per typical (1400-eV) x-ray photon absorbed in the given neutral-particle mix by using the relations

$$(S^+;i) = a_i f_i^{\alpha_i} + b' f_i^{\beta_i} , \quad (12)$$

with b' given by Equation (A13) and a_i , b_i , α_i , and β_i by Table A-1.

Group-1 Step 3. Sum the ions $(S^+;i)$ from each of the species i :

$$S_T = \sum_i (S^+;i) . \quad (13)$$

Group-1 Step 4. Normalize the quantities $(S^+;i)$ to a per-ion-pair basis:

$$(S^+;i)_{ip} = (S^+;i) / S_T . \quad (14)$$

Group-1 Step 5. Determine the ion species per ion pair with account of the dissociative-ionization fractions,

$$R_{N^+} = 0.192 \quad \text{and} \quad R_{O^+} = 0.302 . \quad (15)$$

Group-1 Step 5.1. For the initial photoabsorption events in N_2 and O_2 , let P_{N^+} and P_{O^+} be the number of N^+ and O^+ ions per ion pair, respectively:

$$P_{N^+} = 2f_{N_2} / S_T \quad (16a)$$

$$P_{O^+} = 2f_{O_2} / S_T . \quad (16b)$$

Group-1 Step 5.2. For the subsequent electron slowing-down,
let

$$\begin{aligned}(S^+; e, N_2)_{ip} &= \text{sum of } N^+ \text{ and } N_2^+ \text{ ions per ion pair} \\ &= (S^+; N_2)_{ip} - P_{N^+}\end{aligned}\quad (17a)$$

$$\begin{aligned}(S^+; e, O_2)_{ip} &= \text{sum of } O^+ \text{ and } O_2^+ \text{ ions per ion pair} \\ &= (S^+; O_2)_{ip} - P_{O^+}.\end{aligned}\quad (17b)$$

Group-1 Step 5.3. The number of N^+ , O^+ , N_2^+ , and O_2^+ ions per ion pair are:

$$(N^+)_{ip} = (S^+; N)_{ip} + P_{N^+} + (S^+; e, N_2)_{ip} R_{N^+} \quad (18a)$$

$$(O^+)_{ip} = (S^+; O)_{ip} + P_{O^+} + (S^+; e, O_2)_{ip} R_{O^+} \quad (18b)$$

$$(N_2^+)_{ip} = (S^+; e, N_2)_{ip} (1 - R_{N^+}) \quad (18c)$$

$$(O_2^+)_{ip} = (S^+; e, O_2)_{ip} (1 - R_{O^+}) . \quad (18d)$$

Group-1 Step 6. Determine the newly-formed ion-species densities corresponding to the ion-pair density:

$$\delta_1[N^+] = (N^+)_{ip} IP \quad (19a)$$

$$\delta_1[O^+] = (O^+)_{ip} IP \quad (19b)$$

$$\delta_1[N_2^+] = (N_2^+)_{ip} IP \quad (19c)$$

$$\delta_1[O_2^+] = (O_2^+)_{ip} IP . \quad (19d)$$

One may verify, by use of Equations (18), (17), (14), and (13), that the sum of Equations (19a) through (19d) is just IP.

Group-1 Step 7. Collate the corresponding changes in neutral-particle densities resulting from the ionizing events.

$$\delta_{1i}[N] = IP[(S^+;e,N_2)_{ip}R_{N^+} - (S^+;N)_{ip}] \quad (20a)$$

$$\delta_{1i}[O] = IP[(S^+;e,O_2)_{ip}R_{O^+} - (S^+;O)_{ip}] \quad (20b)$$

$$\delta_{1i}[N_2] = - IP[(S^+;N_2)_{ip} - 0.5P_{N^+}] \quad (20c)$$

$$\delta_{1i}[O_2] = - IP[(S^+;O_2)_{ip} - 0.5P_{O^+}] \quad (20d)$$

To demonstrate that nitrogen and oxygen nuclei are conserved in this treatment of ion production in x-ray deposition, we write

$$\begin{aligned} \delta(N \text{ nuc.}) &\equiv \delta(\text{nitrogen nuclei}) \\ &= \delta_1[N^+] + 2\delta_1[N_2^+] + \delta_{1i}[N] + 2\delta_{1i}[N_2] \end{aligned} \quad (21a)$$

and use Equations (19a), (19c), (20a), (20c), and (17a):

$$\begin{aligned} \delta(N \text{ nuc.}) &= IP[(N^+)_{ip} + 2(N_2^+)_{ip}] + \delta_{1i}[N] + 2\delta_{1i}[N_2] \\ &= IP[(S^+;N)_{ip} + P_{N^+} + (S^+;e,N_2)_{ip}R_{N^+} \\ &\quad + (S^+;e,N_2)_{ip}(1-R_{N^+})2 \\ &\quad - (S^+;N)_{ip} + (S^+;e,N_2)_{ip}R_{N^+} \\ &\quad + P_{N^+} - (S^+;N_2)_{ip}2] \\ &= IP[P_{N^+} + (S^+;e,N_2)_{ip} - (S^+;N_2)_{ip}]2 \\ &= IP[0.0]2 \end{aligned} \quad (21b)$$

A corresponding set of equations and conservation obtain for oxygen nuclei.

Group-1 Step 8. Record the additional changes in neutral-particle densities due to collisional dissociation:

$$\delta_{\text{lni}}[\text{N}] = 2F_d(\text{N}_2) \underbrace{(1-R_{\text{N}+}) (S^+; e, \text{N}_2)_{\text{ip}}}_{\text{collisional ionizations}} \underbrace{\text{IP}}_{\text{collisional dissociations}} \quad (22a)$$

$$\delta_{\text{lni}}[\text{O}] = 2F_d(\text{O}_2) (1-R_{\text{O}+}) (S^+; e, \text{O}_2)_{\text{ip}} \text{IP} \quad (22b)$$

$$\delta_{\text{lni}}[\text{N}_2] = - 0.5\delta_{\text{lni}}[\text{N}] \quad (22c)$$

$$\delta_{\text{lni}}[\text{O}_2] = - 0.5\delta_{\text{lni}}[\text{O}] . \quad (22d)$$

Group 1 Step 9. Sum the changes in N, O, N₂, and O₂ densities due to the ionizing events and collisional dissociation:

$$\delta_1[\text{N}] = \delta_{\text{li}}[\text{N}] + \delta_{\text{lni}}[\text{N}] \quad (23a)$$

$$\delta_1[\text{O}] = \delta_{\text{li}}[\text{O}] + \delta_{\text{lni}}[\text{O}] \quad (23b)$$

$$\delta_1[\text{N}_2] = \delta_{\text{li}}[\text{N}_2] + \delta_{\text{lni}}[\text{N}_2] \quad (23c)$$

$$\delta_1[\text{O}_2] = \delta_{\text{li}}[\text{O}_2] + \delta_{\text{lni}}[\text{O}_2] . \quad (23d)$$

- 7.2 Treat the Group-3 particle according to the basic procedure described in Section A-3. Equation (A33) relates the decrease in CO₂ density to that of N₂. The exponent in Equation (A33), F(α), given by Equation (A29), depends on the mean value of the fractional ionization, estimated from the following equations:

$$\alpha_o = [e]_o / ([e]_o + \text{SMNEUT}) \quad (24a)$$

$$[e]_f = [e]_o + \text{IP} \quad (24b)$$

$$\alpha_f = [e]_f / ([e]_f + \text{SMNEUT} - \text{IP}) \quad (24c)$$

$$\alpha = 0.5(\alpha_o + \alpha_f) . \quad (24d)$$

The total ionization allocated to Group-1 and Group-3 is iteratively distributed between Group-1 and Group-3. Temporarily save the initial value of $\delta_1[\text{N}_2]$, $(\delta_1[\text{N}_2])_o$.

Evaluate Equation (A33):

$$\delta_3[\text{CO}_2] = -[\text{CO}_2]_o [1 - \{([\text{N}_2]_o + \delta_1[\text{N}_2])/[\text{N}_2]_o\}^{F(\alpha)}] \quad (25a)$$

$$\delta_3[\text{CO}_2]_m = -\delta_3[\text{CO}_2] \quad (25b)$$

Assume that a fraction $1/(1+c)$ of the decrease in CO_2 density, $\delta_3[\text{CO}_2]_m$, is due to ionizing reactions.

$$I_3 = \delta_3[\text{CO}_2]_m / (1+c) \quad (26)$$

The ion-pair density I_3 exceeds the ion-pair density originally allocated to Group-3, AIPX_3 . Assume this excess in ion-pair density, ΔI , can be made up at the expense of the much larger density of Group-1 ions:

$$\Delta I = I_3 - \text{AIPX}_3 \quad (27)$$

The new value of AIPX_1 is the old value multiplied by the fraction F given by

$$F = 1 - \Delta I / \text{AIPX}_1 \quad (28)$$

The iterated value of the decrease in N_2 density is

$$\delta'_1[\text{N}_2] = F(\delta_1[\text{N}_2])_o \quad (29)$$

This procedure can be repeated several times to obtain a satisfactory convergence.

When a satisfactory value of F is adopted, one imposes charge conservation to compute the following:

$$\Delta I = \text{AIPX}_1 (1-F) \quad (30a)$$

$$I_3 = \text{AIPX}_3 + \Delta I \quad (30b)$$

$$\delta_3[\text{CO}_2]_m = I_3 (1+c) \quad (30c)$$

7.3 Record the iterated values of the changes in Group-1 species densities by multiplying each of the original values by F.

7.4 Complete the following six steps in treating the Group-1 particles.

Group-1 Step 10. Partition the total change in O_2 among the X- and a-states of O_2 by scaling in proportion to the initial densities.

$$\delta_1[O_2(X)] = \delta_1[O_2] [O_2(X)]_0 / [O_2]_0 \quad (31a)$$

$$\delta_1[O_2(a)] = \delta_1[O_2] \{1 - [O_2(X)]_0 / [O_2]_0\} . \quad (31b)$$

Group-1 Step 11. Record the new densities of X- and a-states of O_2 .

$$[O_2(X)]_1 = [O_2(X)]_0 + \delta_1[O_2(X)] \quad (32a)$$

$$[O_2(a)]_1 = [O_2(a)]_0 + \delta_1[O_2(a)] .$$

Group-1 Step 12. Compute the collisional excitation of $O_2(X)$ to $O_2(a)$. By using Equation (A26) and (A27) we have:

$$x \equiv [O]_0 / [O_2]_0 \quad (33a)$$

$$y \equiv \{O_2(a)/O_2^+\}_{ion\ pair} \quad (33b)$$

$$= \begin{cases} 4.8 & , x < 0.6528 \\ 3.486 x^{-3/4} & , x \geq 0.6528 \end{cases} \quad (33c)$$

$$[O_2(a)]_{ce} = y \delta_1[O_2^+] . \quad (33d)$$

Group-1 Step 13. Record the new (tentative) densities of the X- and a-states of O_2 .

$$[O_2(X)]_2 = [O_2(X)]_1 - [O_2(a)]_{ce} \quad (34a)$$

$$[O_2(a)]_2 = [O_2(a)]_1 + [O_2(a)]_{ce} . \quad (34b)$$

Group-1 Step 14. Limit the number of $O_2(a)$ excitations if the $O_2(X)$ density would be depleted, i.e., if

$$\Delta[O_2(X)] \equiv 0.9[O_2(X)]_1 - [O_2(a)]_{ce} < 0, \quad (35a)$$

use

$$[O_2(a)]_{ce} = 0.9[O_2(X)]_1 \quad (35b)$$

to recompute $[O_2(X)]_2$ and $[O_2(a)]_2$.

Group-1 Step 15. Partition the N atoms into the ground and two excited states (actually, terms). (See Section A-2.3.)

$$\delta_1[N(^4S)] = 0.471 \delta_1[N] \quad (36a)$$

$$\delta_1[N(^2D)] = 0.353 \delta_1[N] \quad (36b)$$

$$\delta_1[N(^2P)] = 0.176 \delta_1[N] . \quad (36c)$$

7.5 Record the densities of the Group-3 product species (see Table 4-4) associated with (a) the ionizing events and (b) the collisional dissociation events and then combine the densities for O and CO.

$$\delta_3[O]_i = I_3 \quad (37a)$$

$$\delta_3[CO]_i = I_3 F_1 \quad (37b)$$

$$\delta_3[O^+]_i = I_3 \cdot 0.5b \quad (37c)$$

$$\delta_3[e]_i = \delta_3[O^+]_i \quad (37d)$$

$$\delta_3[C]_i = \delta_3[O^+]_i \quad (37e)$$

$$\delta_3[CO]_{ni} = I_3^c \quad (38a)$$

$$\delta_3[O]_{ni} = I_3^c \quad (38b)$$

Table 4-4. Prompt-chemistry reactions assumed during x-ray deposition for the Group-3 particle.

Reaction		Branching Ratio*	Number of Ionizing Reactions, cm^{-3}
$\text{CO}_2 \rightarrow$	$\text{CO}_2^+ + e \rightarrow \text{CO} + \text{O}$	a	I_3
	$\text{O} + \underbrace{\text{CO}^+ + e}_{\text{C} + \text{O}}$	b/2	
	$\text{CO} + \text{O}^+ + e$	b/2	
	$\text{CO} + \text{O}$	c	

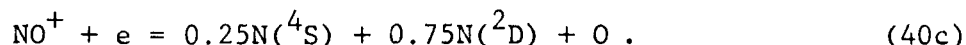
*See Table 4-2.

$$\delta_3[\text{O}] = \delta_3[\text{O}]_i + \delta_3[\text{O}]_{ni} \quad (39a)$$

$$\delta_3[\text{CO}] = \delta_3[\text{CO}]_i + \delta_3[\text{CO}]_{ni} \quad (39b)$$

8. Compute the increased atom densities and decreased electron density from imposing dissociative recombination of those molecular ions (N_2^+ , NO^+ , O_2^+) produced by Group-X deposition and carried in the HAG chemistry.

The total changes in densities of the molecular ions N_2^+ , NO^+ , and O_2^+ from Groups 1 and 2 are $\{\delta_1[\text{N}_2^+] + 0\}$, $\{0 + \delta_2[\text{NO}^+]\}$, and $\{\delta_1[\text{O}_2^+] + \delta_2[\text{O}_2^+]\}$. The assumed dissociative recombination reactions are:



Thus the increased atom densities from dissociative recombination are:

$$\Delta_{\text{N}_2}[\text{N}(^4\text{S})] = \delta_1[\text{N}_2^+] \quad (41a)$$

$$\Delta_{\text{N}_2}[\text{N}(^2\text{D})] = \delta_1[\text{N}_2^+] \quad (41b)$$

$$\Delta_{\text{NO}}[\text{N}(^4\text{S})] = 0.25\delta_2[\text{NO}^+] \quad (41c)$$

$$\Delta_{\text{NO}}[\text{N}(^2\text{D})] = 0.75\delta_2[\text{NO}^+] \quad (41d)$$

$$\Delta_{\text{NO}}[\text{O}] = \delta_2[\text{NO}^+] \quad (41e)$$

$$\Delta_{\text{O}_2}[\text{O}] = 2\{\delta_1[\text{O}_2^+] + \delta_2[\text{O}_2^+]\} \quad (41f)$$

The change in electron density is:

$$\Delta[e] = -\{\delta_1[\text{N}_2^+] + \delta_2[\text{NO}^+] + \delta_1[\text{O}_2^+] + \delta_2[\text{O}_2^+]\} \quad (41g)$$

9. Collate all species densities after Group-X deposition and aforesaid dissociative recombination of molecular ions:

$$[N(^4S)]_{xf} = [N(^4S)]_0 + \delta_1[N(^4S)] + \delta_{N_2}[N(^4S)] \\ + \delta_2[N(^4S)] + \Delta_{NO}[N(^4D)] \quad (42a)$$

$$[N(^4S)]_{xf} = [N(^2D)]_0 + \delta_1[N(^2D)] + \delta_{N_2}[N(^2D)] \\ + \Delta_{NO}[N(^2D)] \quad (42b)$$

$$[N(^2P)]_{xf} = [N(^2P)]_0 + \delta_1[N(^2P)] \quad (42c)$$

$$[N_2]_{xf} = [N_2]_0 + \delta_1[N_2] \quad (42d)$$

$$[NO]_{xf} = [NO]_0 + \delta_2[NO] \quad (42e)$$

$$[NO_2]_{xf} = [NO_2]_0 + \delta_2[NO_2] \quad (42f)$$

$$[O]_{xf} = [O]_0 + \delta_1[O] + \Delta_{NO}[O] + \Delta_{O_2}[O] \\ + \delta_2[O] + \delta_3[O] \quad (42g)$$

$$[O_2(X)]_{xf} = [O_2(X)]_2 + \delta_2[O_2] \quad (42h)$$

$$[O_2(a)]_{xf} = [O_2(a)]_2 \quad (42i)$$

$$[O_3]_{xf} = [O_3]_0 + \delta_2[O_3] \quad (42j)$$

$$[CO]_{xf} = [CO]_0 + \delta_2[CO] + \delta_3[CO] \quad (42k)$$

$$[CO_2]_{xf} = [CO_2]_0 + \delta_3[CO_2] \quad (42l)$$

$$[H]_{xf} = [H]_0 + \delta_2[H] \quad (42m)$$

$$[OH]_{xf} = [OH]_0 + \delta_2[OH] \quad (42n)$$

$$[\text{HO}_2]_{\text{xf}} = [\text{HO}_2]_0 + \delta_2[\text{HO}_2] \quad (42\text{o})$$

$$[\text{H}_2\text{O}]_{\text{xf}} = [\text{H}_2\text{O}]_0 + \delta_2[\text{H}_2\text{O}] \quad (42\text{p})$$

$$[\text{He}]_{\text{xf}} = [\text{He}]_0 \quad (42\text{q})$$

$$[\text{N}^+]_{\text{xf}} = [\text{N}^+]_0 + \delta_1[\text{N}^+] + \delta_2[\text{N}^+] \quad (42\text{r})$$

$$[\text{N}_2^+]_{\text{xf}} = [\text{N}_2^+]_0 \quad (42\text{s})$$

$$[\text{NO}^+]_{\text{xf}} = [\text{NO}^+]_0 \quad (42\text{t})$$

$$[\text{O}^+]_{\text{xf}} = [\text{O}^+]_0 + \delta_1[\text{O}^+] + \delta_2[\text{O}^+] + \delta_3[\text{O}^+] \quad (42\text{u})$$

$$[\text{O}_2^+]_{\text{xf}} = [\text{O}_2^+]_0 \quad (42\text{v})$$

$$[\text{e}]_{\text{xf}} = [\text{e}]_0 + \text{AIPX} + \Delta[\text{e}] - \{\text{AIPX}_2 - \delta_2[\text{e}]\} \\ - \{\text{I}_3 - \delta_3[\text{e}]_i\} . \quad (42\text{w})$$

10. Sum the final densities of N, O, C, and H nuclei, followed by finding the fractional increases in the final values relative to the initial values, as measures of conservation errors in treating the Group-X deposition. One can show analytically, as well as numerically in the code, that the nuclei are conserved. To test charge balance, divide the difference of the final values of positive charge density and electron density by the electron density.

4.4 IONIZATION, SPECIES DENSITIES, AND RESULTANT PRESSURE FROM GROUP-U DEPOSITION

In computing the species from Group-U deposition, we consider three cases, just as we did in Subroutine PHEAT:

- Case 1: B-edge radius (SRR(2)) is smaller than the target-cell entry radius (SR).
- Case 2: B-edge (SRR(2)) is greater than the target-cell exit radius (SRN).
- Case 3: B-edge radius (SRR(2)) is between the target-cell entry radius (SR) and the exit radius (SRN).

The total attenuation factors (FSIGU(J)) are computed from the summed products of Group-U fluences ($F(L) \equiv \text{FLUX}(L)$, photons/cm²) and cross sections (SIGU(L,J), cm²). (Recall that the Group-U fluences computed in Subroutine PHEAT are effective fluences, consistent with the absorbed energy computed as the difference of the (steradianal) energy entering and leaving the cell.) The total attenuation factors are

$$\lambda(J) \equiv \text{FSIGU}(J) = \sum_{L=1}^5 F(L) \times \text{SIGU}(L,J) , \quad J = 1,17 . \quad (43)$$

The attenuation factors for ionization per se of N₂, O₂(X), and O₂(a) are obtained by subtracting terms for dissociation:

$$\lambda_i(1) = \lambda(1) - \text{SIGU}(1,1)F(1) \quad (44a)$$

$$\lambda_i(2) = \lambda(2) - \text{SIGU}(1,2)F(1) \quad (44b)$$

$$\lambda_i(9) = \lambda(9) - \text{SIGU}(1,9)F(1) . \quad (44c)$$

The total survival probability of species J is

$$P(J) \equiv \text{PROBSU}(J) = e^{-\lambda(J)} . \quad (45)$$

The branching ratios a_1 , a_2 , and a_9 for N₂⁺, O₂⁺, and O₂⁺ production from N₂, O₂(X), and O₂(a), respectively, are

$$a_1 = \lambda_i(1)/\lambda(1) \quad (46a)$$

$$a_2 = \lambda_i(2)/\lambda(2) \quad (46b)$$

$$a_9 = \lambda_i(9)/\lambda(9) . \quad (46c)$$

SIGU(L,J) is the absorption cross-section of Species J for Subgroup-L photons, given in Tables 4-5a, 4-5b, and 4-5c. The currently adopted values are in the columns headed Vol. 17-1 (and entered as data in Block Data BLOCKH) and may be compared (where there are corresponding species) with the values used for ROSCOE-Radar in the columns headed Vol. 17. The reactions considered for Group-U deposition, including instantaneous dissociative recombination of all

Table 4-5a. UV photoabsorption cross-sections (N_2, O_2).

UV Benchmark ^b											
ROSCOE Group No.	Sa-75a Group No.	Bin Edges, eV	Source and Mulc. No.	Photon Energy, eV	λ , Å	$\sigma(N_2)$, Mb			$\sigma(O_2)$, Mb		
						HL-73a	HL-73b	Vol. 17-1	HL-73a	HL-73b	Vol. 17-1
1	1	8.00	NV,1	9.99	1240.1	0			1.5		
			NII,1	11.42	1085.1	0			2		
			OIV,1	11.99	1033.8	0			0.95		
			NIII,1	12.51	990.98	2.5 ^e	0.0	1.4	2.9	2.45	2.6
			NII,2	13.53	916.34	10.3 ^e	1.6	0	5.8	5.8	2
2	2	13.62	OIII,1	14.85	834.5	7.7 ^e			13.9 ^e		
				14.86			4.4			15.5	
			OII,1	14.87	832.8	6.5 ^e		8	17.1 ^e		20
			OII,3	15.55	796.661	10.6	10.6		24.9	24.9	
			OIV,1	15.70	789.36	20.9 ^e	20.9		27.1 ^e	27.1	
3	3	15.85	NII,4	15.97	775.957	114	114		16.3	16.3	
			NIV,1	16.20	765.14	76	76	20	24.9	24.9	22
			NIII,2	16.23	764.01	22 ^e			20.6		
				16.42			25.2		20.1		
			NII,8	16.59	746.976	29.4			19.5		
4	4	16.93	Seven Multiplets				30		23.7		
			Eighteen Multiplets				24.9	25			25
			Eleven Multiplets				13.3		15.6		
								20			20

Table 4-5b. UV photoabsorption cross-sections ($N(^4S)$, $N(^2D)$, $N(^2P)$, O, NO).

ROSCOE Group Number	UV Bench- mark Group Number	$\sigma(N(^4S))$			$\sigma(N(^2D))$		$\sigma(N(^2P))$	
		HL-73b	Vol. 17-1	Vol. 17 ^d	HL-73b	Vol. 17-1	HL-73b	Vol. 17-1
1	1	0	0	0	4.5	4.3	4.85	6.2
	2	0			4.1		7.6	
2	3	10.2	10.4	10	9.95	9.7	8.6	9.8
	4	10.7			9.3		10.9	
3	5	10.7	10.9	10	9.4	10.0	10.9	10.9
	6	10.9			9.4		10.9	
	7	11.0			10.6		10.8	
4	8	11.0	11.1	10	10.6	9.7	10.8	9.8
	9	11.3			10.3		10.46	
5	10	10.9	5.9	10	9.1	2.6	9.1	4.0
	11	5.9			2.6		4.0	

ROSCOE Group Number	UV Bench- mark Group Number	$\sigma(O)$			$\sigma(NO)$	
		HL-73b	Vol. 17-1	Vol. 17 ^d	HL-73b	Vol. 17-1
1	1	0	0	0	10.3	20
	2	0			28.9	
2	3	2.8	2.9	3.2	21.0	19
	4	2.9			17.8	
3	5	3.0	3.1	3.2	23.1	21
	6	3.1			10.8	
	7	3.1			33.1	
4	8	3.2	8.5	9	17.3	21
	9	7.4			19.2	
5	10	9.6	7.6	9	23.3	23
	11	7.6			22.5	

Table 4-5c. UV photoabsorption cross-sections (NO_2 , $\text{O}_2(^1\Delta_g)$, O_3 , H, H_2O , OH, HO_2 , CO_2 , He).

ROSCOE Group Number	$\sigma(\text{NO}_2)$		$\sigma(\text{O}_2(^1\Delta_g))$		$\sigma(\text{O}_3)$		$\sigma(\text{H})$	
	Vol. 17-1	Ref.	Vol. 17-1	Ref.	Vol. 17-1	Ref.	Vol. 17-1	Ref.
1	20	SH-66a	2.6	(g)	~10	SH-66a	0	
2	19	(f)	20	(g)	23	SH-66a	5.3	PK-76c
3	21	(f)	22	(g)	34	SH-66a	4.0	PK-76c
4	21	(f)	24	(g)	27	SH-66a	1.8	(i)
5	23	(f)	16	(g)	9	(h)	~0	(i)

ROSCOE Group Number	$\sigma(\text{H}_2\text{O})$		$\sigma(\text{OH})$		$\sigma(\text{HO}_2)$		$\sigma(\text{CO}_2)$	
	Vol. 17-1	Ref.	Vol. 17-1	Ref.	Vol. 17-1	Ref.	Vol. 17-1	Ref.
1	9	SH-66a	9	(k)	7	(l)	14	(m)
2	16.5	SH-66a	17	(k)	18	(l)	21	(m)
3	16	SH-66a	16	(k)	19	(l)	35.8	(m)
4	14	(j)	14	(k)	19	(l)	31.5	(m)
5	7	(j)	7	(k)	11	(l)	21.5	(m)

ROSCOE Group Number	$\sigma(\text{CO})$		$\sigma(\text{He})$	
	Vol. 17-1	Ref.	Vol. 17-1	Ref.
1	~25 ⁽ⁿ⁾	SH-66a	0	
2	~35 ^(o)	SH-66a	0	
3	~30 ^(p)	SH-66a	0	
4	30	SH-66a LC-73	~0	HK-71
5	12	LC-73	4	HK-71

Footnotes for Tables 4-5a, 4-5b, and 4-5c:

- (a) Sa-75a quotes bin edges at 6.2, 13.6, 15.6, 17, 30, and 82 eV.
- (b) HL-73b, Section 2.3.2.
- (c) Multiplets included in the photodeposition code FOTOKEM [HL-73a]; multiplet number from WS-66.
- (d) Volume 17 of The ROSCOE Manual, quoting Table A-1 of FS-73 (in turn from DD-70b).
- (e) Variation in cross sections for multiplet lines is large.
- (f) No data are available at wavelengths below $\sim 1000 \text{ \AA}$; therefore, we assumed $\sigma(\text{NO}_2) \approx \sigma(\text{NO})$.
- (g) No data are available for $\text{O}_2(^1\Delta_g)$; therefore we assumed $\sigma(\text{O}_2(^1\Delta_g)) \approx \sigma(\text{O}_2)$.
- (h) Based on extrapolation of data in SH-66a.
- (i) Based on extrapolation of data in PK-76c.
- (j) In SH-66a, data between 195 and 1085 \AA of J. Romand (private communication) are given. The absolute values of these data are significantly higher than those obtained by Watanabe and Jursa [1964] or Metzger and Cook [1964a] as reported in Hu-71b. To obtain $\sigma(\text{H}_2\text{O})$ listed, the data of J. Romand were averaged and scaled to the values of Metzger and Cook.
- (k) No data are available for OH; therefore we assumed $\sigma(\text{OH}) \approx \sigma(\text{H}_2\text{O})$.
- (l) No data are available for HO_2 ; therefore we assumed $\sigma(\text{HO}_2) \approx 0.5[\sigma(\text{O}_2) + \sigma(\text{OH})] \approx 0.5(\sigma(\text{O}_2) + \sigma(\text{H}_2\text{O}))$.
- (m) Derived from measurements reported in SH-66a and LC-73.
- (n) Cross sections range from about 0 to as large as 160 Mb in the wavelength range of Group 1.
- (o) Cross sections range from about 15 to 120 Mb in the wavelength range of Group 2.
- (p) Cross sections range from about 15 to 60 Mb in the wavelength range of Group 3.

molecular ions, are given in Table 4-6.

To facilitate writing the differential equations for the changes in species densities during the Group-U deposition, we introduce the following notation.

$$S(J) = \lambda(J)/F \quad (47a)$$

$$\equiv \sum_{L=1}^5 \text{SIGU}(L,J)f(L) \quad (47b)$$

where $f(L)$ = fractional spectral fluence

$$= dF(L)/dF$$

$dF(L)$ = differential fluence of Subgroup-L photons

dF = differential total fluence.

The differential equations for the species densities during the Group-U deposition are:

$$d[N_2]/dF = -[N_2]S(1) \quad (48a)$$

$$d[O_2(X)]/dF = -[O_2(X)]S(2) + [O_3]S(10) \quad (48b)$$

$$d[N(^2S)]/dF = -[N(^4S)]S(3) + 2\beta_1[N_2]S(1) + \beta_2[NO]S(7) \quad (48c)$$

$$\begin{aligned} d[O]/dF = & -[O]S(4) + 2[O_2(X)]S(2) + [NO]S(7) \\ & + [NO_2]S(8) + 2[O_2(a)]S(9) + [O_3]S(10) \\ & + [OH]S(12) + [HO_2]S(13) + [CO_2]S(15) \\ & + [CO]S(16) \end{aligned} \quad (48d)$$

$$\begin{aligned} d[N(^2D)]/dF = & -[N(^2D)]S(5) + 2(1 - \beta_1)[N_2]S(1) \\ & + (1 - \beta_2)[NO]S(7) \end{aligned} \quad (48e)$$

Table 4-6. Reactions for Group-U deposition.

Species Number	Reaction*			UV Subgroup-L
1	N_2	$\rightarrow \left\{ \begin{array}{l} N_2^+ + e \rightarrow \end{array} \right.$	$2\beta_1 N(^4S) + 2(1 - \beta_1) N(^2D)$ $2\beta_1 N(^4S) + 2(1 - \beta_1) N(^2D)$	1 2,5
2	$O_2(X)$	$\rightarrow \left\{ \begin{array}{l} O_2^+ + e \rightarrow \end{array} \right.$	$O + O$ $O + O$	1 2,5
3	$N(^4S)$	\rightarrow	$N^+ + e$	2,5
4	O	\rightarrow	$O^+ + e$	2,5
5	$N(^2D)$	\rightarrow	$N^+ + e$	1,5
6	$N(^2P)$	\rightarrow	$N^+ + e$	1,5
7	NO	$\rightarrow NO^+ + e \rightarrow$	$\beta_2 N(^4S) + (1 - \beta_2) N(^2D) + O$	1,5
8	NO_2	$\rightarrow NO_2^+ + e \rightarrow$	$NO + O$	1,5
9	$O_2(a)$	$\rightarrow \left\{ \begin{array}{l} O_2^+ + e \rightarrow \end{array} \right.$	$O + O$ $O + O$	1 2,5
10	O_3	$\rightarrow \left\{ \begin{array}{l} O_3^+ + e \rightarrow \end{array} \right.$	$O_2(X) + O$ $O_2(X) + O$	1 2,5
11	H	$\rightarrow H^+ + e \rightarrow$	H	2,5
12	OH	$\rightarrow \left\{ \begin{array}{l} OH^+ + e \rightarrow \end{array} \right.$	$O + H$ $O + H$	1 2,5
13	HO_2	$\rightarrow \left\{ \begin{array}{l} HO_2^+ + e \rightarrow \end{array} \right.$	$OH + O$ $OH + O$	1 2,5

(continued)

Table 4-6. (Cont'd)

Species Number		Reaction				UV Subgroup-L
14	H_2O	$\rightarrow \left\{ \begin{array}{l} OH \\ HO_2^+ + e \rightarrow \end{array} \right.$	OH	+	H	1
			OH	+	H	2,5
15	CO_2	$\rightarrow \left\{ \begin{array}{l} CO \\ CO_2^+ + e \rightarrow \end{array} \right.$	CO	+	O	1
			CO	+	O	2,5
16	CO	$\rightarrow \left\{ \begin{array}{l} C \\ CO^+ + e \rightarrow \end{array} \right.$	C	+	O	1
			C	+	O	2,5
17	He	$\rightarrow He^+ + e \rightarrow$		He		5

* $\beta_1 = 0.5$, $\beta_2 = 0.25$.

$$d[N(^2P)]/dF = -[N(^2P)]S(6) \quad (48f)$$

$$d[NC]/dF = -[NO]S(7) + [NO_2]S(8) \quad (48g)$$

$$d[NO_2]/dF = -[NO_2]S(8) \quad (48h)$$

$$d[O_2(a)]/dF = -[O_2(a)]S(9) \quad (48i)$$

$$d[O_3]/dF = -[O_3]S(10) \quad (48j)$$

$$d[H]/dF = -[OH]S(12) + [H_2O]S(14) \quad (48k)$$

$$d[OH]/dF = -[OH]S(12) + [HO_2]S(13) + [H_2O]S(14) \quad (48l)$$

$$d[HO_2]/dF = -[HO_2]S(13) \quad (48m)$$

$$d[H_2O]/dF = -[H_2O]S(14) \quad (48n)$$

$$d[CO_2]/dF = -[CO_2]S(15) \quad (48o)$$

$$d[CO]/dF = -[CO]S(16) \quad (48p)$$

$$d[He]/dF = 0 \quad (48q)$$

After introducing the following notation, we write the solutions to the differential equations.

$$G(J,K) \equiv G(\lambda, P, J, K)$$

$$\equiv PCFUN(\lambda, P, J, K)$$

$$= [P(K) - P(J)]\lambda(K)/[\lambda(J) - \lambda(K)] \quad (49)$$

$$\begin{aligned}
H(I,J,K) &\equiv H(\lambda,P,I,J,K) \\
&\equiv \text{PCFUNC}(\lambda,P,I,J,K) \\
&= \frac{\lambda(I)G(K,J) - \lambda(J)G(K,I)}{\lambda(I) - \lambda(J)} \quad (50)
\end{aligned}$$

PCFUN and PCFUNC appear as function routines in the code.

$$[N_2]_{uf} = [N_2]_{xf} P(1) \quad (51a)$$

$$[O_2(X)]_{uf} = [O_2(X)]_{xf} P(2) + [O_3]_{xf} G(2,10) \quad (51b)$$

$$\begin{aligned}
[N(^4S)]_{uv} &= [N(^4S)]_{xf} P(3) + \beta_2 [NO]_{xf} G(3,7) \\
&\quad + 2\beta_1 [N_2]_{xf} G(3,1) + \beta_2 [NO_2]_{xf} H(7,8,3) \quad (51c)
\end{aligned}$$

$$\begin{aligned}
[O]_{uv} &= [O]_{xf} P(4) + 2[O_2(X)]_{xf} G(4,2) + [NO]_{xf} G(4,7) \\
&\quad + [NO_2]_{xf} \{G(4,8) + H(7,8,4)\} + 2[O_2(a)]_{xf} G(4,9) \\
&\quad + [O_3]_{xf} \{G(4,10) + 2H(2,10,4)\} + [OH]_{xf} G(4,12) \\
&\quad + [HO_2]_{xf} \{G(4,13) + H(12,13,4)\} + [CO]_{xf} G(4,16) \\
&\quad + [CO_2]_{xf} \{G(4,15) + H(16,15,4)\} + [H_2O]_{xf} H(12,14,4) \quad (51d)
\end{aligned}$$

$$\begin{aligned}
[N(^2D)]_{uv} &= [N(^2D)]_{xf} P(5) + (1-\beta_2)[NO]_{xf} G(5,7) \\
&\quad + 2(1-\beta_1)[N_2]_{xf} G(5,1) + (1-\beta_2)[NO_2]_{xf} H(7,8,5) \quad (51e)
\end{aligned}$$

$$[N(^2P)]_{uf} = [N(^2P)]_{xf} P(6) \quad (51f)$$

$$[\text{NO}]_{\text{uf}} = [\text{NO}]_{\text{xf}} P(7) + [\text{NO}_2]_{\text{xf}} G(7,8) \quad (51g)$$

$$[\text{NO}_2]_{\text{uf}} = [\text{NO}_2]_{\text{xf}} P(8) \quad (51h)$$

$$[\text{O}_2(\text{a})]_{\text{uf}} = [\text{O}_2(\text{a})]_{\text{xf}} P(9) \quad (51i)$$

$$[\text{O}_3]_{\text{uf}} = [\text{O}_3]_{\text{xf}} P(10) \quad (51j)$$

For hydrogen, set $\lambda(11) = 0$ and $P(11) = 1$.

$$\begin{aligned} [\text{H}]_{\text{uf}} = & [\text{H}]_{\text{xf}} + [\text{OH}]_{\text{xf}} G(11,12) + [\text{H}_2\text{O}]_{\text{xf}} \{G(11,14) \\ & + H(14,12,11)\} + [\text{HO}_2]_{\text{xf}} H(13,12,11) \end{aligned} \quad (51k)$$

$$[\text{OH}]_{\text{uf}} = [\text{OH}]_{\text{xf}} P(12) + [\text{HO}_2]_{\text{xf}} G(12,13) + [\text{H}_2\text{O}]_{\text{xf}} G(12,14) \quad (51l)$$

$$[\text{HO}_2]_{\text{uf}} = [\text{HO}_2]_{\text{xf}} P(13) \quad (51m)$$

$$[\text{H}_2\text{O}]_{\text{uf}} = [\text{H}_2\text{O}]_{\text{xf}} P(14) \quad (51n)$$

$$[\text{CO}_2]_{\text{uf}} = [\text{CO}_2]_{\text{xf}} P(15) \quad (51o)$$

$$[\text{CO}]_{\text{uf}} = [\text{CO}]_{\text{xf}} P(16) + [\text{CO}_2]_{\text{xf}} G(16,15) \quad (51p)$$

$$[\text{He}]_{\text{uf}} = [\text{He}]_{\text{xf}} \quad (51q)$$

For carbon, set $\lambda(C) = 0$, $P(C) = 1$.

$$[\text{C}]_{\text{uf}} = [\text{C}]_{\text{xf}} + [\text{CO}]_{\text{xf}} G(C,16) + [\text{CO}_2]_{\text{xf}} H(15,16,C). \quad (51r)$$

To maximize the ionization at early time, as suggested by W. Knapp, we re-establish the molecular ions produced and dissociatively recombined by the Group-X and -U depositions (and allow the molecular

ion decay to be predicted by the later-time chemistry module). First, record the densities of the molecular ions N_2^+ , NO^+ , and O_2^+ which underwent dissociative recombination during Group-U deposition.

$$[N_2^+]_u = a_1 \{ [N_2]_{xf} - [N_2]_{uf} \} \quad (52a)$$

$$[NO^+]_u = [NO]_{xf} \{ 1 - P(7) \} \quad (52b)$$

$$[O_2^+]_u = a_2 \{ [O_2(X)]_{xf} - [O_2(X)]_{uf} \} + a_9 \{ [O_2(a)]_{xf} - [O_2(a)]_{uf} \} . \quad (52c)$$

Next, add in the corresponding ions from the Group-X deposition.

$$[M_1^+]_d \equiv [N_2^+]_d = \delta_1 [N_2^+] + [N_2^+]_u \quad (53a)$$

$$[M_2^+]_d \equiv [NO^+]_d = \delta_2 [NO^+] + [NO^+]_u \quad (53b)$$

$$[M_3^+]_d \equiv [O_2^+]_d = \delta_1 [O_2^+] + \delta_2 [O_2^+] + [O_2^+]_u . \quad (53c)$$

We must subtract the products of dissociative recombination from the appropriate species densities, with the constraint that N and O atom densities remain non-negative. If limiting is required, maintain the fractional contributions and scale appropriately.

The total density of these molecular ions is

$$[M^+]_d = \sum_{i=1}^3 [M_i^+]_d \quad (54)$$

and the fractional contributions by each of the ions is

$$f_i = [M_i^+]_d / [M^+]_d , \quad i = 1, 3 . \quad (55)$$

For the dissociative recombination reactions for N_2^+ , NO^+ , and O_2^+ (see Table 4-6), let R_1 , R_2 , and R_3 be the number of $N(^4S)$, $N(^2D)$, and O atoms produced per dissociative recombination with fractional

contributions by N_2^+ , NO^+ , and O_2^+ of f_1 , f_2 , and f_3 . Then

$$R_1 = 2\beta_1 f_1 + \beta_2 f_2 \quad (56a)$$

$$R_2 = 2(1-\beta_1)f_1 + (1-\beta_2)f_2 \quad (56b)$$

$$R_3 = f_2 + 2f_3 \quad (56c)$$

For a total density of dissociative recombination equal to $[M^+]_d$, the densities of the product atomic species are

$$S_{id} = [M^+]_d R_i, \quad i=1,3 \quad (57)$$

The tentative final values for these atomic-species densities are

$$S_{iuf} = S_{iuv} - S_{id}, \quad i=1,3 \quad (58)$$

where S_{iuv} is given by Equation (51c), (51e), and (51d) for $i = 1, 2, 3$, respectively. If $S_{iuf} > 1$ for each of the three atomic species, no revision is required; otherwise, a new value of $[M^+]_d$ is determined:

$$[M^+]_d = \text{Min} \left\{ \begin{array}{ll} (S_{iuv} - 1)/R_i, & S_{iuv} > 1 \\ 0.5 S_{iuv}/R_i, & S_{iuv} \leq 1 \end{array} \right\} \quad (59)$$

Then, revised values are computed for S_{id} , S_{iuf} , and

$$[M_i^+]_d = [M^+]_d f_i, \quad i=1,3 \quad (60)$$

The final molecular-ion densities are

$$[M_i^+]_{uf} = [M_i^+]_{xf} + [M_i^+]_d, \quad i=1,3 \quad (61)$$

There are two equivalent ways of obtaining the atomic-ion densities. One is to solve the differential equations and the other is to appropriately difference the neutral species densities. The results of the two methods can be reconciled by adding and subtracting appropriate terms, followed by regrouping. Here we present the results from the second method.

$$\begin{aligned}
[N^+]_{uf} = & [N^+]_{xf} + [N(^4S)]_{xf} - [N(^4S)]_{uv} \\
& + [N(^2D)]_{xf} - [N(^2D)]_{uv} + [N(^2P)]_{xf} - [N(^2P)]_{uf} \\
& + [NO]_{xf} - [NO]_{uf} + [NO_2]_{xf} - [NO_2]_{uf} \\
& + 2\{[N_2]_{xf} - [N_2]_{uf}\} \quad (62)
\end{aligned}$$

$$\begin{aligned}
[O^+]_{uf} = & [O^+]_{xf} + [O]_{xf} - [O]_{uv} + [NO]_{xf} - [NO]_{uf} \\
& + [OH]_{xf} - [OH]_{uf} + [CO]_{xf} - [CO]_{uf} + [H_2O]_{xf} \\
& - [H_2O]_{uf} + 2\{[O_2(X)]_{xf} - [O_2(X)]_{uf} + [O_2(a)]_{xf} \\
& - [O_2(a)]_{uf} + [NO_2]_{xf} - [NO_2]_{uf} + [HO_2]_{xf} - [HO_2]_{uf} \\
& + [CO_2]_{xf} - [CO_2]_{uf}\} + 3\{[O_3]_{xf} - [O_3]_{uf}\} \quad (63)
\end{aligned}$$

The final electron density is

$$[e]_{uf} = [N^+]_{uf} + [O^+]_{uf} + \sum_{i=1}^3 [M_i^+]_{uf} \quad (64)$$

There remains the task of devising a truly satisfactory procedure for computing a pressure increment in addition to that computed in Subroutine PHEAT. The treatment in Subroutine PHEAT is incomplete because the Group-U subgroups are deposited independently of each other across an appreciable path length without accounting for either species depletion by other subgroups or additional absorbers resulting from the (instantaneous) dissociative recombination that is included in Subroutine PCHEM. (Note, however, that the partial heating computed in Subroutine PHEAT does serve the purpose of defining effective fluences for the Group-U subgroups that are used in Subroutine PCHEM.) Any additional pressure increment computed in Subroutine PCHEM must be consistent with (1) that computed in Subroutine PHEAT and with (2) the return of pressure computed by the later-time chemistry in CHEMEF. The problem is further complicated by the re-establishment of the molecular

ions produced by the Group-X and Group-U depositions. To compensate for (1) removing a number of N and O atoms (whose sum is $2[M^+]_d$, consisting of $S_{1d} N(^4S)$ atoms, $S_{2d} N(^2D)$ atoms, and $S_{3d} O$ atoms) at temperature T_{old} , (2) establishing a number $[M^+]_d$ of molecular ions at temperature T_{new} and a number $[M^+]_d$ of electrons at temperature T_{ef} , and (3) returning energies (in eV) of

$$E(N_2^+) = 15.58 - 9.76 - 2(1-\beta_1)2.37 = 3.45 \quad (65a)$$

$$E(O_2^+) = 12.06 - 5.12 = 6.94 \quad (65b)$$

$$E(NO^+) = 9.27 - 6.51 - (1-\beta_2) 2.37 = 0.9825 \quad (65c)$$

each time a re-established N_2^+ , O_2^+ , and NO^+ ion dissociatively recombines, we should subtract an amount of thermal energy equal to

$$[M^+]_d \{1.5k(T_{new} + T_{ef} - 2T_{old}) + \bar{E}_d\} \text{ eV/cm}^3, \quad (66)$$

where

$$\bar{E}_d = E(N_2^+)f_1 + E(O_2^+)f_2 + E(NO^+)f_3. \quad (67)$$

However, as an interim approximation we shall account for only ΔP given by

$$\Delta P = -[M^+]_d \bar{E}_d 1.6 \times 10^{-12} \text{ erg/cm}^3 \quad (68)$$

$$P_1 = P_{old} + \Delta P. \quad (69)$$

To ensure that the heavy-particle pressure will always be positive, we have added the electron pressure (computed below) to the previously-found value for the total pressure. This interim measure needs to be reviewed and improved.

To compute the temperature TEF taken to be common to the thermal electrons, the N_2 vibrational states, and the $O(^1D)$ -to- $O(^3P)$ population ratio, we use the GET-prepared Subroutine TEXK [Vol. 11] which determines such a temperature when given $[N_2]$, $[O]$, $[e]$, and the energy per cubic centimeter (ET) to be divided among the three modes.

As an interim measure we compute ET from

$$ET = 2 \times \delta[e]_{x,u} + \delta[e]_{HP} \times E_{pe}$$

where $\delta[e]_{x,u}$ is the incremental electron density produced by the Group-X and -U depositions, the factor 2 is an interim assumption for the energy in the three modes per newly-formed electron in the Group-X and -U depositions, $\delta[e]_{HP}$ is the incremental electron density produced by the heavy-particle depositions, and E_{pe} is the sum of the electron thermal and $O(^1D)$ excitation energies per newly-formed electron in the heavy-particle deposition, obtained from Subroutine HPCHEM.

Sum the final densities of N, O, C, and H nuclei, followed by finding the fractional increases in the final values relative to the initial values, as measures of conservation errors in treating the Group-U deposition.

The foregoing describes the combined treatment of target cells that are Case 1 or Case 3. For Case 1, the treatment is complete, but for Case 3, the final cell properties are determined by volume-weighting the two portions, one of which is inside the B-edge and the other is outside the B-edge.

For Case 2, the entire cell is inside the B-edge and the only remaining species are assumed to be N^+ , O^+ , and e. The temperature of both electrons and heavy particles is taken to be 1 eV.

The final step in Subroutine PCHEM is to store the cell quantities in temporary storage BUF1 until the loop over the entire column of target cells is completed, after which the entire column of cell quantities is transferred to scratch storage in large-core memory. After the energy deposition is completed for the entire grid, cell quantities in the scratch area are transferred to Time-Slot 2.

SECTION 5

REFERENCES

- BB-74a C.A. Blank, M.H. Bortner, T. Baurer, and A.A. Feryok, "A Pocket Manual of the Physical and Chemical Characteristics of the Earth's Atmosphere," DNA 3467H, 1 July 1974.
- CI-72 CIRA-1972, "COSPAR International Reference Atmosphere, 1972" Compiled by COSPAR Working Group A, Akademie-Verlag, Berlin, 1972.
- DD-70b T.N. Delmer, E.P. dePlomb, et al., "Effects of High Altitude Nuclear Explosions," DASA 2593 (Gulf Radiation Technology Gulf-RT-11010), 28 October 1970.
- FS-71a F.E. Fajen and D. Sappenfield, "Single-Burst Weapon Effects Calculations for Altitudes Between 97 and 250 km," Los Alamos Scientific Laboratory Report LA-4606, June 1971.
- FS-73 F.E. Fajen, D.S. Sappenfield, R.W. Moore, "Studies in High-Altitude Weapon Phenomenology," DNA 3100T (MRC-R-48), June 1973.
- Gi-74 F.R. Gilmore, "Preliminary Revised Production Rate Distribution for Bombarded Air," letter 28 May 1974, R&D Associates.
- HK-71 R.D. Hudson and L.J. Kieffer, "Compilation of Atomic Ultraviolet Photoabsorption Cross Sections for Wavelengths between 3000 and 10 Å, Atomic Data 2, 205 (1971).
- HL-73a D.A. Hamlin, R.W. Lowen, B.F. Myers, M.R. Schoonover, and J.I. Valerio, "Theoretical High-Altitude Nuclear-Explosion Studies, Vol. 1: Generation and Deposition of Radiation from Debris-Air Pistons; Phenomenology of MK-12 Events," DNA 3216F-1 (SAI-73-220-LJ), 15 May 1974.
- HL-73b D.A. Hamlin, R.W. Lowen, B.F. Myers, M.R. Schoonover, and J.I. Valerio, "Theoretical High-Altitude Nuclear-Explosion Studies, Vol. 2: Resonance Trapping, Deposition, and Resulting Chemistry of Ultraviolet Radiation; Energy Deposition of Heavy Particles," DNA 3216F-2 (SAI-73-220-LJ), 15 May 1974.
- HM-72b D.A. Hamlin, B.F. Myers, and M.R. Schoonover, "Studies of High-Altitude Nuclear-Induced Optical-Infrared Radiation," DNA 3012F (SAI-72-238-LJ), February 1973.
- HS-75b D.A. Hamlin, M.R. Schoonover, J.I. Valerio, J.Y. Wang, "The ROSCOE Manual Volume 17 - High-Altitude Debris-Energy Deposition," DNA 3964F-17 (SAI-75-609-LJ-5), 22 September 1975.

- Hu-71b R.D. Hudson, "Critical Review of Ultraviolet Photoabsorption Cross Sections for Molecules of Astrophysical and Aeronomic Interest," Rev. of Geophys. and Space Phys. 9, 305 (1971).
- LC-73 L.C. Lee, R.W. Carlson, D.L. Judge, and M. Ogawa, "The Absorption Cross Sections of N_2 , O_2 , CO, NO, CO_2 , N_2O , CH_4 , C_2H_6 , and C_4H_{10} from 180 to 700 Å, J. Quant. Spectrosc. Radiat. Transfer 13, 1023 (1973).
- MS-75 B.F. Myers and M.R. Schoonover, "Electron Energy Degradation in the Atmosphere: Consequent Species and Energy Densities, Electron-Flux and Radiation Spectra," DNA 3513T (SAI-74-619-LJ), 3 January 1975.
- MS-76a B.F. Myers and M.R. Schoonover, "UV Photon and Electron Deposition in the Atmosphere," DNA 4068F (SAI-76-696-LJ), 2 August 1976.
- PK-76c H.P. Palenius, J.L. Kohl, and W.H. Parkinson, "Absolute Measurement of the Photoionization Cross Section of Atomic Hydrogen with a Shock Tube for the Extreme Ultraviolet," Phys. Rev. A13, 1805 (1976).
- Sa-75a D.S. Sappenfield, "Ultraviolet Radiation Rate Constants and Yields for High-Altitude Nuclear Explosions," DNA 3849T (MRC-R-220), October 1975.
- SH-66a J.O. Sullivan and A.C. Holland, "A Congeries of Absorption Cross Sections for Wavelengths Less than 3000 Å, NASA CR-371, January 1966.
- SK-75 T.L. Stephens and A.L. Klein, "Electron Energy Deposition in the Atmosphere," Vol. I, GE75TMP-7, General Electric TEMPO, Center for Advanced Studies, Santa Barbara, California, May 1975.
- SS-72d T. Sawada, D.J. Strickland, and A.E.S. Green, "Electron Energy Deposition in CO_2 ," J. Geophys. Res. 77, 4812 (1972).
- WS-66 W.L. Wiese, M.W. Smith and B.M. Glennon, "Atomic Transition Probabilities, Vol. I. Hydrogen Through Neon," National Standard Reference Data Series, National Bureau of Standards Number 4, 20 May 1966.

APPENDIX A

SPECIES FROM X-RAY DEPOSITION

A-1 INTRODUCTION

A procedure for calculating the species formed following x-ray deposition is presented. This procedure is generally an improvement over that in ROSCOE-Radar of assuming ions (of neutral species) are formed in proportion to the densities of neutral species [HS-75b, p. 108]. Here we take account of, not only collisional ionization, but also dissociative ionization, collisional dissociation, collisional excitation, and the dependence of ion production on arbitrary mixes of the neutral species. In addition, a more accurate estimate of the CO_2 loss resulting from x-ray deposition is given.

A-2 PRINCIPAL SPECIES FORMATION

In this section we will initially consider ion production from N_2 , O_2 , and O as absorbers; later, we include N as an absorber and, in some parts of the calculation, NO . (The full treatment of NO and eight other minor species is discussed in Section 4.) Later in this section we consider the neutral species from non-ionizing collisions of the slowing-down electrons.

To predict the ion species resulting from x-ray deposition, we modify the relations between ion species and fractional neutral density previously developed [MS-76a] for photon absorption. These relations are of the form [cf. MS-76a, Equation (16)]

$$(S^+;i) = a_i f_i^{\alpha} + b_i f_i^{\beta} (E_p - E_p^0) \quad (\text{A1})$$

where $(S^+;i)$ is the number of ions formed from absorber i per photon absorbed in the neutral-particle mix of N_2 , O_2 , and O . For molecular absorbers, $(S^+;i)$ is the sum of the resulting molecular and atomic ions, assumed to be singly charged. The quantities a , b , α , β , and E_p^0 are constants [MS-76a, Table 6, p. 36], E_p is the energy of the

absorbed photon, and f_i is the fractional density of absorber i among the neutral species. In MS-76a, the values of the constants were developed for the neutral species N_2 , O_2 , and O on the basis of photon deposition results computed for ambient atmospheres with compositions given by the CIRA-1972 mean atmosphere [CI-72] corresponding to the range of altitudes from 60 to 250 km and for photon energies E_p of 33.67 eV and larger. These constants are reproduced here in Table A-1.

In using Equation (A1) for present purposes, we need to address three problems: (a) extending the use of Equation (A1) for photon energies greater than 281 eV, (b) extending the use of Equation (A1) for chemically-altered atmospheres, and (c) incorporating N atoms as absorbers.

A-2.1 Ion Formation Following High-Energy Photon Absorption in an Ambient Atmosphere

The derivation of Equation (A1) and the constants of Table A-1 were based on calculations in which the maximum photon energy was 281 eV [MS-76a]. To calculate and verify the accuracy of the ions per absorbed photon at higher photon energies, we take two steps. Firstly, we compute the ions per absorbed photon using Equation (A1) but excluding the ions formed in the x-ray absorption event. Thus, the counted ions per absorbed photon result from the slowing-down of a photoelectron formed in the x-ray absorption event. Such ions per absorbed photon are shown to be accurate by comparison with detailed calculations [MS-75, MS-76a] on the slowing-down of high-energy electrons. Secondly, we modify Equation (A1) to include the results of the x-ray absorption event for photon energies above 281 eV.

Equation (A1) was derived from calculations of the absorption of photons with energies below the K-absorption edge of both N and O atoms. According to the x-ray deposition model previously formulated [MS-75, Appendix B], the absorption event in this case resulted in one electron and one ion. Therefore, to use Equation (A1) to describe only the effect of the photoelectron slowing-down, it must be modified as follows:

$$(S^+;i)' = (S^+;i) - f_i \quad (A2)$$

Table A-1. Constants used in Equation (A1) relating absorber and species formed per absorbed photon [MS-76a, Table 6].

Absorber i^a	a_i	b_i	α_i	β_i	E_p° , eV
N_2	1.06	0.0266	0.872	0.649	33.67
O_2	1.26	0.0238	0.927	0.821	33.67
O	1.20	0.0350	1.09	1.30	33.67

^a Later, in Section A-2.2.3 when we add nitrogen atoms as absorbers, we shall postulate that the constants for N are the same as those for O.

Here, $(S^+;i)^-$ is the number of ions formed from absorber i per photoelectron and $(S^+;i)$ and f_i are as defined above. The use of f_i as opposed to the accurate quantity, $\sigma_i f_i / \sum \sigma_i f_i$ (where σ_i is the photoabsorption cross-section), is an approximation which introduces an error of less than 5 percent in the case of the slowing down of a 900-eV photoelectron. Equation (A2) will now be tested for higher-energy (>281 eV) photons against the detailed calculations [MS-75, MS-76a].

To use Equation (A2) in the comparison with the detailed calculations, the contributions of atomic and molecular ions to Equation (A2) must be separated. This separation is accomplished with the following relationships:

$$R_N^+ \equiv (N^+) / [(N^+) + (N_2^+)] = 0.184 + 5.8 \times 10^{-5} (z-60) \quad (A3)$$

$$\approx 0.192 \text{ for } z = 200 \text{ km}$$

and

$$R_O^+ \equiv (O^+) / [(O^+) + (O_2^+)] = 0.302 \quad (A4)$$

where z is the altitude (km). Both of these equations are based on calculations of electron slowing-down [MS-76a, Tables 10a-10d]. Equation (A3) gives (within about 2 percent) the ratio of the N^+ ions to the total ions derived from N_2 for incident electron energies in the range from 230 to 900 eV and for atmospheric compositions corresponding to the range of altitudes from 60 to 250 km. (See Tables 10a, 10b, 10c, and 10d of MS-76a.) Equation (A4) gives the ratio of the O^+ ions to the total ions derived from O_2 , averaged over the range of incident electron energies from 230 to 900 eV.

In making the comparison between the predictions of Equation (A2) and the detailed calculations [MS-76a], we consider a range of energies of the x-ray photon and the incident electron. For the detailed calculations [MS-76a], the selected range for the incident electrons is from 230 to 900 eV; for the calculations based on Equation (A2), the selected range for the incident photons is from 650 to 1400 eV. For this latter range, the photon energy will be above the K-absorption-edge energy for N and O atoms and will, generally, yield photoelectrons having energies within the range used in the detailed calculations. However, the ranges of energies are not explicitly considered in the comparison since the quantity compared, the ion species per ion pair, does not vary significantly over the energy range specified for either the detailed calculations or those based on Equation (A2). The variation is generally not greater than 5 percent in the former calculations and generally not greater than 1 percent in the latter calculations.

The results of the calculations are given in Table A-2A in terms of the ion species per ion pair. This quantity is calculated from Equation (A2) by forming the ratio

$$(S^+; i)_{IP} \equiv (S^+; i) / \sum_i (S^+; i) \quad (A5)$$

The entries are averages over the energy ranges cited above for the detailed calculations and those based on Equation (A2). For all comparisons, the relative error is not greater than about 16 percent; for the majority of cases, the relative error is less than 9 percent.

Table A-2. Comparison of predictions using Equation (A2) with earlier, detailed calculations.

A. Comparison of ion species per ion pair (columns 2 and 3)

Species	60 km			110 km		
	Eq. (A2)	MS-76a ^a	% Error	Eq. (A2)	MS-76a ^a	% Error
N ₂ ⁺	0.632	0.629	0.5	0.611	0.624	-2.1
N ⁺	0.142	0.142	0.0	0.141	0.143	-1.4
O ₂ ⁺	0.158	0.156	1.3	0.102	0.091	12.1
O ⁺	0.068	0.073	-6.8	0.147	0.143	2.8

Species	145 km			250 km		
	Eq. (A2)	MS-76a ^a	% Error	Eq. (A2)	MS-76a ^a	% Error
N ₂ ⁺	0.459	0.502	-8.6	0.198	0.217	-8.8
N ⁺	0.107	0.117	-8.5	0.048	0.052	-7.7
O ₂ ⁺	0.053	0.051	3.9	0.012	0.013	-7.7
O ⁺	0.382	0.330	15.8	0.741	0.719	3.1

B. Comparison of electron volts per ion pair (for 900-eV electrons)

	Altitude (km)			
	60	110	145	250
E _{ip} (pe) ^c	34.8	35.5	32.8	28.1
E _{ip} (e) ^d	34.5	34.1	32.5	29.2

^a Results for 60-, 110-, 145-, and 250-km altitude are obtained from an average over the range $230 < U(\text{eV}) < 900$ of the results from Tables 10a, 10b, 10c, and 10d, respectively, in MS-76a.

^b % error = $\{[\text{Eq. (A2)}] - (\text{MS-76a})\} / (\text{MS-76a}) \times 100$.

^c Calculated by using $E_{ip}(\text{pe}) = 900 / (\sum_i (S^+; i) - 1)$; also see Equation (19) of MS-76a.

^d From Table 11a of MS-76a for $U = 900$ eV.

In Table A-2B, values of the electron volts per ion pair, E_{ip} , are given for the detailed calculations ($E_{ip}(e)$) and those based on Equation (A2) ($E_{ip}(pe)$). For this comparison, both the photoelectron in the x-ray absorption case and the incident electron in the detailed calculation had an energy of 900 eV. The agreement is adequate. There is some unevenness in the $E_{ip}(pe)$ values as a function of altitude and this is attributed to the compromises in the fitting of the parameters in Equation (A1) to the data from the detailed calculations [MS-76a] on photon absorption.

From the above calculations and comparisons, we find Equation (A2) to be satisfactory in computing the ion densities resulting from photoelectron slowing-down in ambient atmospheres following absorption of x-rays with energies of 650 eV and larger.

The ion species per ion pair in the given neutral-particle mix, $(S^+)_{ip}$, resulting from absorption of x-rays with energies above 650 eV, are given by the following equations:

$$(N_2^+)_{ip} = [(S^+; N_2) - 2f_{N_2}]R_{N_2^+}/IP \quad (A6)$$

$$(N^+)_{ip} = [(S^+; N_2)R_{N^+} + 2f_{N_2}R_{N_2^+}]/IP \quad (A7)$$

$$(O_2^+)_{ip} = [(S^+; O_2) - 2f_{O_2}]R_{O_2^+}/IP \quad (A8)$$

$$(O^+)_{ip} = [(S^+; O_2)R_{O^+} + 2f_{O_2}R_{O_2^+} + (S^+; O)]/IP \quad (A9)$$

where

$$IP = \sum_i (S^+; i) \quad (A10)$$

$$R_{N_2^+} = 1 - R_{N^+} \quad (A11a)$$

$$R_{O_2^+} = 1 - R_{O^+} \quad (A11b)$$

In Equations (A6) through (A9), the factor 2 arises from the assumption that in the photoabsorption event two atomic ions and two photoelectrons are formed from each molecular absorber per absorbed photon.

In Table A-3 we compare the results obtained from Equations (A6) through (A9) with (a) the detailed calculations modified to account for an x-ray absorption event (by adding the ion corresponding to the photoelectron) and with (b) the ion species obtained from the prescription used in ROSCOE-Radar [HS-75b]. The new method of calculating the ion species per ion pair, Equations (A6) through (A9), is shown in Table A-3 to be a generally better approximation to the detailed calculations than the older prescription [HS-75b]. Table A-3 applies to absorptions in ambient atmospheres (in contrast to a chemically-disturbed atmosphere considered in Section A-2.2).

Equations (A6) through (A9) depend on the photon energy, E_p , through Equation (A1). However, for the number of ions per ion pair the dependence on photon energy is sufficiently weak, provided E_p is greater than 650 eV, to justify eliminating this dependence. If E_p in Equation (A1) is fixed at 1400 eV, then, for photon energies greater than 650 eV, the error in calculating the ion species from the specialized equation will not exceed about 10 percent compared with accounting for the energy dependence. Making this simplification leads to the following equation:

$$(S^+; i)_{ip} = (a_i f_i^{\alpha i} + b'_i f_i^{\beta i}) / IP \quad (A12)$$

where

$$b'_i = 1366 b_i \quad (A13)$$

A-2.2 Ion Formation in Chemically-Disturbed Atmospheres

To calculate the ion species per ion pair in chemically-disturbed atmospheres, consideration must be given to the altered composition as compared with ambient atmospheres.

Table A-3. Comparison of ion species per ion pair calculated according to (a) the new method, (b) the detailed method [MS-76a], and the older ROSCOE-Radar method [HS-75b].^a

z, km	Method	$(N_2^+)_\text{ip}$	% E ^b	$(N^+)_\text{ip}$	% E	$(O_2^+)_\text{ip}$	% E	$(O^+)_\text{ip}$	% E
60	new	0.618	1.3	0.156	-2.5	0.154	0.7	0.072	-7.7
	detailed	0.610		0.160		0.153		0.078	
	old	0.790	29.5	0.000	-100	0.210	37.3	3×10^{-6}	-100
110	new	0.597	-2.0	0.155	-3.7	0.099	10.0	0.148	5.0
	detailed	0.609		0.161		0.090		0.141	
	old	0.730	19.9	0.000	-100	0.120	33.3	0.150	6.4
145	new	0.450	-9.5	0.117	-10.7	0.052	~0.0	0.381	19.4
	detailed	0.497		0.131		0.052		0.319	
	old	0.526	7.3	0.000	-100	0.059	15.7	0.415	30.1
250	new	0.194	-12.2	0.051	-12.0	0.012	-8.3	0.743	4.8
	detailed	0.221		0.058		0.013		0.709	
	old	0.183	-17.2	0.000	-100	0.012	-8.3	0.805	13.5

^a The ion species per ion pair derived from the new method apply strictly to a 1400-eV x-ray photon; the results presented here for the detailed method have been averaged over those for 450-eV and 900-eV photoelectrons and take account of the x-ray absorption event (by adding the ion corresponding to the photoelectron). These two calculations are regarded as comparable since, for the photoelectron slowing-down, the resulting ion species per photoelectron are insensitive to the photoelectron energy, at least for energies of 450 eV and larger.

^b % E = percent error = $\{[(\text{new or old}) - (\text{detailed})]/(\text{detailed})\} \times 100$. Note that with this definition a negative error is formally limited to -100%.

A-2.2.1 Effect of Ambient Electrons

The effect of ion formation, due to thermal electron densities significantly greater than ambient values, has been determined [MS-76a, pp. 61,63,64] for high-energy electron deposition. For high-energy electrons (450 and 900 eV), the ion species per ion pair were changed by less than about 10 percent for electron densities 10^4 times the ambient value at altitudes in the range from 100 to 250 km and about 10^{11} times the ambient value at 60 km. At the upper limit to the electron density in these studies, the steady-state approximation for the electron energy distribution, used in the calculations, became invalid because of the loss of non-thermal electrons via dissociative recombination. Maintaining the validity of the steady-state approximation limited the ratio of thermal electrons to neutrals at 60, 110, and 145 km to 1.5×10^{-4} , 5×10^{-4} , and 3×10^{-2} , respectively; at 250 km, an electron density of 10^4 times the ambient value corresponded to an average of 2.6 free electrons per neutral particle. However, at 250 km, where the ratio of thermal electrons to neutrals was not significantly limited, the change in ion species per ion pair was of the order of 10 percent or less; thus, it is reasonable to assume that species formation by electron or photon deposition is not strongly affected by an increased electron density even up to 72 percent ionization at all altitudes considered.

A-2.2.2 Effect of Ambient Ions

The effect on ion formation, due to ion densities significantly greater than ambient values, has not been determined. A simple prescription to partially account for their effect is developed here.

Consider the disturbed atmosphere to consist of an ion gas (of singly-ionized particles) and a neutral gas. The fraction of the x-ray energy deposited in the neutral gas will be modeled by assuming that the probability that an electron expends energy on a target particle is proportional to the number density of the particle, inversely proportional to its ionization energy I (or dissociation energy, for molecular ions), and inversely proportional to its effective mean excitation energy \bar{E} defined by the expression

$$g \equiv \frac{1}{\bar{E}/I} = \frac{E_{ip}}{I} - 1 \quad (A14)$$

where E_{ip} is the energy expended (eV) in forming an ion pair within the given particle gas. For neutral and ion gases consisting of atomic and molecular species, the portion of the total energy deposited per unit volume, E_d , which is assigned to the neutral gas, E_{dn} , is given by

$$E_{dn}/E_d \equiv f_n = \frac{\sum_n T_n}{\sum_n T_n + \sum_i T_i} \quad (A15)$$

where

$$T_n = \frac{[n]}{I_n} (1+g_n) \quad , \quad n = N_2, O_2, NO, N, O \quad (A16)$$

$$T_i = \frac{[i]}{I_i} (1+g_i) \quad , \quad i = N_2^+, O_2^+, NO^+, N^+, O^+ \quad (A17)$$

Values of the parameters entering Equations (A14), (A15), (A16), and (A17) are given in Table A-4. The value of g for the atomic species is taken to be unity; for O , this value is based on the fact that the energy per ion pair in an O gas is about twice the ionization energy [MS-76a] and for N , O^+ , and N^+ , on the assumption of similar values. The value of g for neutral molecules is taken to be $4/3$ on the basis that E_{ip}/I is 2.24 for N_2 and 2.48 for O_2 ; for molecular ions, g is taken to be $3/4$ for N_2^+ and O_2^+ and $4/3$ for NO^+ under the assumption that \bar{E} is about the same as for neutral molecules. An improved basis for assigning these values would certainly be desirable.

A-2.2.3 Addition of Nitrogen Atoms as Absorbers

In chemically-disturbed atmospheres, the density of nitrogen atoms may increase to represent a significant set of absorbers of the x-ray photons. To account for this situation, we add nitrogen atoms to the set of absorbers by modifying Equations (A6) through (A9).

Since calculations of the absorption and slowing-down process have not been performed for atmospheres containing nitrogen atoms, we assume that nitrogen atoms may be treated analogously to oxygen atoms for the purpose of calculating the ion species per ion pair from Equation (A12). In this case Equations (A6), (A8), and (A9) remain

Table A-4. Parameters used in the expressions for partitioning the deposited energy between the neutral and ionized gases.

Species	I^a , eV	g^c	E_{ip}^b , eV/ip
N ₂	15.6	4/3	35
O ₂	12.1	4/3	30
NO	9.27	4/3	25
N	14.5	1	27
O	13.6	1	27
N ₂ ⁺	8.7	3/4	
O ₂ ⁺	6.7	3/4	
NO ⁺	10.8	4/3	
N ⁺	29.6	1	
O ⁺	35.1	1	

^a I is the ionization energy except for the molecular ions for which it is the dissociation energy. Values taken from BB-74a, pp. 84,85.

^b Values of the energy per ion pair are nominal selections from those computed in MS-76a for N₂, O₂, and O. The value for N is assigned to be that for O. The value for NO is a postulated value.

^c See text which discusses the assignment of these values.

unchanged, but Equation (A7) becomes analogous to Equation (A9), i.e.,

$$(N^+)_{ip} = [(S^+; N_2)R_{N^+} + 2f_{N_2}R_{N_2^+} + (S^+; N)]/IP \quad (A7a)$$

where the constants used in Equation (A1) to evaluate $(S^+; O)$ will be taken to be those used to evaluate $(S^+; N)$, and the sum in Equation (A10) is now over the species $i = N_2, O_2, O$, and N .

A-2.2.4 Mean Energy Per Ion Pair

The energy per ion pair used in ROSCOE-Radar [HS-75b, p. 108] to compute the number of ion pairs from the energy deposited is 35 eV/ip. At high altitudes where atomic oxygen dominates the atmospheric composition, the use of this value can introduce an error of about 20 percent. A more accurate value for the energy per ion pair in the neutral gas may be obtained from the prescription

$$\bar{E}_{ip} = \sum_s f_s E_{ip}(s) \quad (A18)$$

where values of $E_{ip}(s)$ are given in Table A-4 for $s = N_2, O_2, NO, N$, and O . In atmospheres without NO and N , Equation (A18) is accurate to within about 3 percent.

A-2.3 Neutral Species Formation from Non-Ionizing Collisions

MS-76a (p. 36) notes that relations similar to Equation (A1) could be developed for neutral species, but that no attempt was made to do so. In the absence of such relations, we shall resort to simpler procedures. We are mainly interested in the atoms formed when slowing-down electrons collisionally dissociate N_2 and O_2 . We shall also consider the excitation of $O_2(a)$ since this species is carried in the late-time chemistry used in the high-altitude grid.

Let F_d denote the ratio of collisional dissociation to collisional ionization, i.e.,

$$F_d(N_2) = \frac{N_2 \text{ collisional dissociation}}{N_2 \text{ collisional ionization}} \quad (A19a)$$

$$F_d(O_2) = \frac{O_2 \text{ collisional dissociation}}{O_2 \text{ collisional ionization}} \quad (A19b)$$

From the data in MS-76a (Tables 10a through 10d) one can infer that, for 900-eV electrons,

$$F_d(N_2) \approx 0.22 \text{ to } 0.31,$$

a range which depends on the way predissociation states are treated. This inferred value of $F_d(N_2)$ was obtained by using the distribution of species per ion pair to evaluate the expression

$$F_d(N_2) = \frac{0.5[\sum_s N(s) - N^+]}{N_2^+} \quad (A20)$$

where $s = {}^4S, {}^2D, {}^2P$.

F. Gilmore has begun a review of the question of predissociation in N_2 and advocates more excited-state nitrogen atoms per ion pair than indicated in MS-76a. Gilmore [DNA IR Data Review Meeting at AFGL, 11 April 1979] suggested 0.9 N^* atoms per ion pair. In a private communication on 23 April 1979, Gilmore stated his review was continuing but that his best guess as of the moment, for the number of nitrogen atoms per ion pair, including dissociative ionization as well as collisional dissociation, was

$$0.8 N({}^4S), \quad 0.6 N({}^2D), \quad \text{and} \quad 0.3 N({}^2P).$$

If we use a value of 0.14 N^+ per ion pair (obtained in MS-75, MS-76a, and SK-75, even though Gi-74 quotes 0.18) and 0.63 N_2^+ ions per ion pair (as obtained in MS-75, MS-76a, and SK-75; Gi-74 quotes 0.62), then

$$F_d(N_2) = \frac{0.5[0.8 + 0.6 + 0.3 - 0.14]}{0.63} = 1.24, \quad (A21)$$

larger than that indicated in MS-76a by a factor of 5.6 to 4.0.

It should be noted that Gilmore's guessed-values are indeed preliminary, and that it seemed he was assuming 0.2 $N({}^4S)$ atoms from dissociative ionization (in contrast to our use of 0.14 $N({}^4S)$). However, this difference doesn't change the value of $F_d(N_2)$ much, as seen from

$$F_d(N_2) = \frac{0.5[0.8 - (0.2-0.14) + 0.6 + 0.3 - 0.14]}{0.63}$$

$$= 1.19. \quad (A22)$$

Though it doesn't change the estimate of $F_d(N_2)$, we note that a possible assignment of dissociating states per ion pair is

$$\begin{aligned} &0.2N(^4S) + 0.2N^+ \\ &0.3N(^4S) + 0.3N(^2D) \\ &0.3N(^4S) + 0.3N(^2P) \\ &0.15N(^2D) + 0.15N(^2D) \end{aligned}$$

We don't know what Gilmore had in mind.

We need a prescription for assigning the relative abundances of the nitrogen atom states. Values inferred by averaging values from MS-76a [Table 10a, p. 57] are

$$\begin{aligned} N(^4S) : N(^2D) : N(^2P) &= 0.217 : 0.266 : 0.0013 \\ &= 0.448 : 0.549 : 0.003 \end{aligned} \quad (A23)$$

From Gilmore's statements we have

$$\begin{aligned} N(^4S) : N(^2D) : N(^2P) &= 0.8 : 0.6 : 0.3 \\ &= 0.471 : 0.353 : 0.176 \end{aligned} \quad (A24)$$

Turning to O_2 , one can infer from the data in MS-76a (Tables 10a through 10d) that for 900-eV electrons,

$$F_d(O_2) = 0.88 \quad (A25)$$

Based on the 900-eV electron results in Tables 10a, b, c, d in MS-76a, one can show that the following fit function is satisfactory:

$$y \equiv \{O_2(a)/O_2^+\}_{\text{ion pair}} \quad (\text{A26a})$$

$$x \equiv [O]/[O_2] \quad (\text{A26b})$$

$$y \equiv \begin{cases} 4.8 & , x < 0.6528 \\ 3.486 x^{-3/4} & , x \geq 0.6528 \end{cases} \quad (\text{A27})$$

A-3 CO₂ LOSS FOLLOWING X-RAY DEPOSITION

The procedure in ROSCOE-Radar for treating the loss of CO₂ following x-ray deposition is to assume the loss is proportional to that of N₂. Here, a more accurate estimate is made by determining the relative loss of CO₂ on the basis of electron flux spectra and known electron energy-loss functions.

The rate of loss of species S, in the framework of an energy bin structure over the energy range, is given by

$$-\frac{d[S]}{dt} = \sum_j \phi(j)L(j,S)[S] \quad (\text{A28})$$

where j is the group number for the energy bins [MS-75, p. 11], $\phi(j)$ is the electron flux per unit energy in energy bin j (electrons cm⁻² sec⁻¹ eV⁻¹), and L(j,S) is the energy-loss function (eV cm² per electron) of species S in energy bin j. The usual energy-loss function has been modified by removing the contribution of processes not leading to CO₂ or N₂ loss. The energy-loss function values are given in Table A-5; the modified values are in parentheses.

Values of the species-loss frequency, $\sum_j \phi(j)L(j,S)$, are given in Table A-6 for various altitudes and electron densities, for both CO₂ and N₂. The electron flux values, $\phi(j)$, used in computing the species-loss frequencies were taken from the calculations in MS-76a (data extracted from the microfiche records of these calculations). The ratio of the species-loss frequency for CO₂ to that for N₂ can be adequately represented by the following expression:

$$\frac{\sum_j \phi(j)L(j,CO_2)}{\sum_j \phi(j)L(j,N_2)} = 1.92 + 0.7 (1 - e^{-1.36\sqrt{\alpha}}) \equiv F(\alpha) \quad (\text{A29})$$

Table A-5. Energy-loss function values for CO₂ and N₂ up to 1 keV.

Electron Energy eV	Loss Function, 10 ⁻¹⁶ cm ² eV	
	CO ₂ ^a	N ₂ ^b
11	∞ ^c	10 (∞) ^c
14	1 (0.9) ^c	13 (0.4)
18	4	14 (3.4)
23	20	22 (12)
29	34	31 (21)
36	50	42 (32)
45	75	52 (40)
57	85	63 (50)
72	100	69 (56)
90	109	71 (58)
110	120	71 (59)
140	121	69 (59)
180	120	63 (54)
230	118	57 (49)
290	109	50 (43)
360	103	45 (39)
450	99	39 (34)
570	87	33 (29)
720	80	27 (24)
900	70	23 (20)

^a SS-72d.

^b MS-76a, p. 62.

^c Energy-loss function excluding processes not leading to loss by target molecule, i.e., energy-loss function for destruction of target molecule.

Table A-6. Values of the species-loss frequency, $F(S)$, for CO_2 and N_2 as a function of altitude, electron density, and photoelectron energy.

Altitude km	$[e]_3^a$ cm ⁻³	Photoelectron Energy eV	$F(CO_2) \equiv$ $\sum \phi(j)L(j, CO_2)$	$F(N_2) \equiv$ $\sum \phi(j)L(j, N_2)$	$F(CO_2)/F(N_2)$
60	1 (10)	900	5.00 (1)	2.61 (1)	1.92
60	1 (12)	900	4.98 (1)	2.59 (1)	1.92
60	1 (10)	450	3.17 (1)	1.66 (1)	1.91
60	1 (12)	450	3.16 (1)	1.66 (1)	1.90
110	1 (5)	900	1.59 (5)	8.09 (4)	1.95
110	1 (9)	900	1.55 (5)	7.89 (4)	1.96
110	1 (5)	450	1.02 (5)	5.28 (4)	1.93
110	1 (9)	450	1.00 (5)	5.19 (4)	1.93
145	2 (5)	900	5.20 (6)	2.62 (6)	1.98
145	2 (9)	900	3.76 (6)	1.69 (6)	2.22
145	2 (5)	450	3.45 (6)	1.77 (6)	1.95
145	2 (9)	450	2.60 (6)	1.24 (6)	2.10
250	6.3 (5)	900	2.02 (8)	9.65 (7)	2.09
250	6.3 (9)	900	1.81 (7)	6.85 (6)	2.64
250	6.3 (5)	450	1.33 (8)	6.62 (7)	2.01
250	6.3 (9)	450	1.07 (7)	4.61 (6)	2.32

^a₁ (10) means 1×10^{10} .

where the fractional ionization, α , is given by

$$\alpha = \frac{[e]}{[e] + \sum_i [i]} \quad , \quad (A30)$$

$[e]$ is the electron number density, and $[i]$ is the density of the i^{th} neutral species. Thus, the fractional change in CO_2 density is related to the fractional change in N_2 density by the expression

$$\frac{d[\text{CO}_2]}{[\text{CO}_2]} = F(\alpha) \frac{d[\text{N}_2]}{[\text{N}_2]} \quad . \quad (A31)$$

If we assume $F(\alpha)$ is constant, determined by some appropriate mean value for α as the N_2 density changes, then we can integrate Equation (A31) to obtain

$$[\text{CO}_2]_f = [\text{CO}_2]_i \{ [\text{N}_2]_f / [\text{N}_2]_i \}^{F(\alpha)} \quad . \quad (A32)$$

Thus, the change in $[\text{CO}_2]$ is

$$\begin{aligned} \delta[\text{CO}_2] &\equiv [\text{CO}_2]_f - [\text{CO}_2]_i \\ &= -[\text{CO}_2]_i (1 - \{ [\text{N}_2]_f / [\text{N}_2]_i \}^{F(\alpha)}) \quad . \end{aligned} \quad (A33)$$

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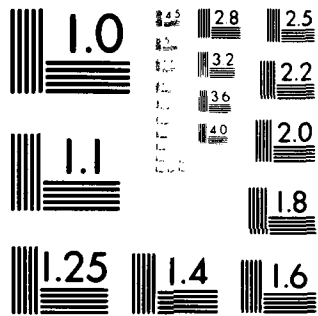


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